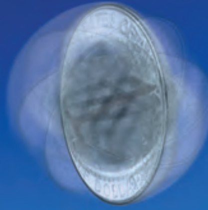
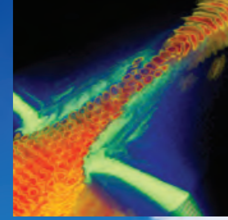
LOS ALAMOS SCIENCE AND TECHNOLOGY MAGAZINE



MARCH 2013



1663

CLEANING UP CARBON

Los Alamos
NATIONAL LABORATORY
EST 1943

1663

LOS ALAMOS SCIENCE AND TECHNOLOGY MAGAZINE

About Our Name:
During World War II, all that the outside world knew of Los Alamos and its top-secret laboratory was the mailing address—P. O. Box 1663, Santa Fe, New Mexico. That box number, still part of our address, symbolizes our historic role in the nation's service.

About the LDRD Logo:
Laboratory Directed Research and Development (LDRD) is a competitive, internal program by which Los Alamos National Laboratory is authorized by Congress to invest in research and development that is both highly innovative and vital to our national interests. Whenever *1663* reports on research that received support from LDRD, this logo appears at the end of the article.

About the Cover:


Even with rapid growth of renewable energy sources, the world will remain dependent on fossil fuels for the foreseeable future. Burning these fuels produces carbon dioxide and other greenhouse gases, which drive increased temperatures and climate change worldwide. The capture and long-term storage of carbon dioxide in deep, geological reservoirs is one possible approach to mitigating these changes but presents challenges in the scale at which it must be done (billions of metric tons per year) and the associated cost. To meet these global challenges, Los Alamos scientists are making advances in virtually every aspect of carbon capture and storage research.

Los Alamos Firsts

Server Science

Paul Ginsparg never intended his "e-print archive" to catalyze a revolution in science communication. It just turned out that way.

Ginsparg was a maverick young theorist at Los Alamos National Laboratory when he conceived of the archive. It was 1991, there was email but no World Wide Web, and in many physics disciplines, new ideas and results were routinely communicated through preprints—abstracts or un-refereed early drafts of papers—which were available months before the corresponding published papers. Researchers spent considerable time and institutional resources preparing, printing, and mailing preprints, but often little time organizing the ones they received (choosing to utilize the ever-popular "paper mound" filing system).

Ginsparg recognized that if researchers simply emailed their preprints to a common site, a computer could automatically extract the content, organize it, store it, and avail it to be read or downloaded. Preprint costs would be obviated, and a structured, searchable archive of breaking research would lay at a subscriber's fingertips.

Such an archive would also, in a sense, level the research playing field. Each institution constructed its own preprint distribution list—those not on it were excluded from the research buzz. But anyone connected to a computer network would be able to access Ginsparg's archive, so everyone from students to Nobel laureates could contribute to the science.

After spending a few summer weekends writing the necessary computer code, Ginsparg launched the system in August of 1991. The whole enterprise ran on a computer that sat beneath his desk. He had envisioned the archive serving a few hundred scientists and receiving roughly 100 full-text submissions per year, but he severely underestimated its cultural impact.

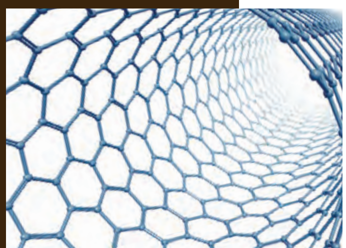
Scientists began using the archive as an unofficial record of scientific activity—even using it to stake claims of intellectual property. Within two years, the archive had evolved into the primary means of daily communication for a global community of researchers.

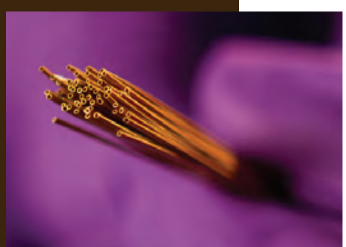
Today, the official "arXiv," (pronounced "archive," on the web at http://arXiv.org) contains close to 800,000 full texts, receives 83,000 new texts each year, and serves roughly a million full-text downloads to about 400,000 distinct users every week. It has broadened to cover most active research fields of physics, astronomy, mathematics, nonlinear sciences, computer science, statistics, and, more recently, parts of biology and even finance. Its role in promulgating science cannot be overestimated.

Paul Ginsparg
CREDIT: CORNELL UNIVERSITY

IN THIS ISSUE

FEATURES





SPOTLIGHT

nanoto

assessing the potential health hazards of nanotechnology

Used in products from sunscreens to solar panels, manufactured nanoparticles are proliferating so quickly that safety testing procedures are struggling to keep up. A revolutionary new approach to bioassessment using artificial human tissues may soon change that.

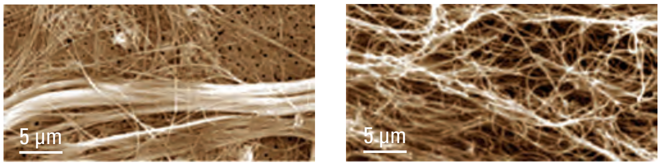
Asbestos was a popular 19th- and early 20th-century addition to building materials, insulation, and fire retardants. To this day, the mineral fibers still hide in walls and ceilings. With the danger of inhaling those tiny needles now well known, it's hard to imagine how asbestos became so ubiquitous.

Now researchers at Los Alamos are among those applying the lessons learned from asbestos's legacy to even smaller particles that are building a modern-day industrial revolution. Nanoparticles come in a huge variety of shapes and chemical compositions, and their applications are equally varied, offering to revolutionize everything from energy production to disease treatment. Already, the little structures populate everyday items like fast food containers, cosmetics, sunscreens, and carbon-composite sports equipment.

As with any other chemical, producing and using engineered nanoparticles at the industrial scale raises questions about the risks of exposing people, like factory workers, who could touch or inhale them. Sorting out the toxicity of carbon tubes, copper spheres, cadmium discs, and roughly a thousand other commercially produced materials between the 1- and 100-nanometer scale hasn't kept pace with their rapidly evolving applications.

oxicity

In the search for more accurate and efficient techniques to evaluate the health hazards of nanoparticles, Los Alamos researchers are developing artificial human tissues and organs to replace animal test subjects.



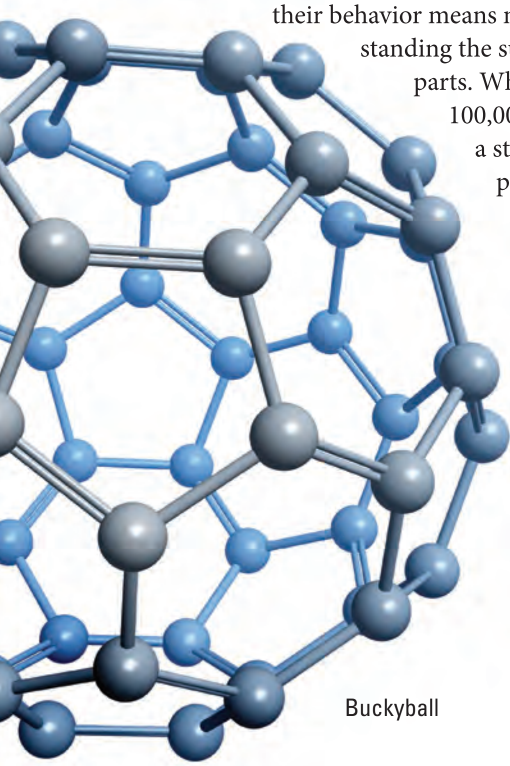
Asbestos (left) and long, multi-walled carbon nanotubes (right) aren't just similar in appearance (shown here under a transmission electron microscope). In a 2008 U.K. study, mice exposed to carbon nanotubes developed inflammation similar to the lung disease caused by asbestos.

CREDIT: KEN DONALDSON, UNIVERSITY OF EDINBURGH

Fortunately, if researchers learn which properties separate a benign nanomaterial from an unsafe one, they can design materials to maximize functionality and minimize health impacts. Biologists and materials scientists at Los Alamos National Laboratory are working in the burgeoning field of nanotoxicology to uncover the harmful properties of tiny particles before the structures further permeate our material lives. Los Alamos scientist Rashi Iyer and her team are developing techniques to rapidly test and even predict which particles are the most damaging to lungs and skin. As they observe the biological impacts of nanomaterials, they are developing lab-grown human tissues and engineering synthetic millimeter-scale organs. In the future, those surrogates could replace animal testing with more relevant technology for evaluating not only the smallest engineered particles, but also many other chemicals, from pharmaceuticals to bioweapons. "We need a new paradigm for toxicity testing of anything, not just nanomaterials," says Iyer.

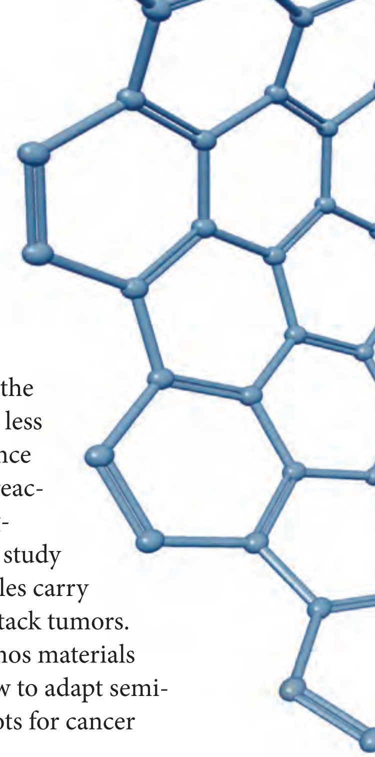
Sizing Up Nanoparticles

Molecular and atomic scale particles are built with elements from all parts of the periodic table, and predicting their behavior means more than understanding the sum of their molecular parts. When particles are about 100,000 times smaller than a strand of human hair, properties like conductivity, optical behavior, and chemical reactivity are different than those of a larger version of the same material. These differences within the same kinds of materials lend special uncertainty to nanoparticle toxicity.



Buckyball

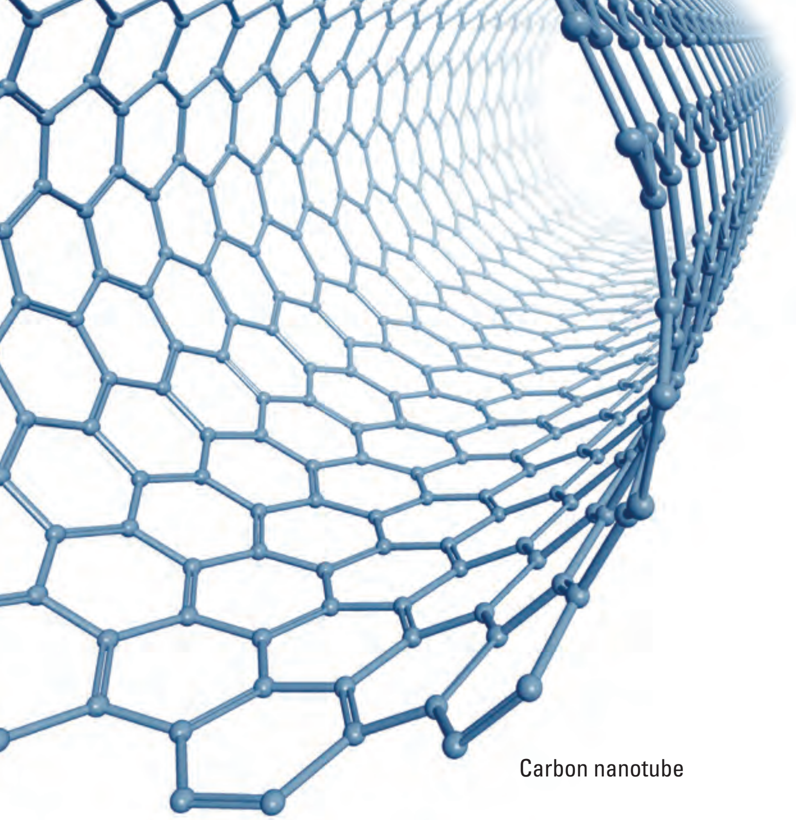
For example, small particle size translates into a higher surface area-to-volume ratio and enhances chemical reactivity, much like granulated sugar dissolving more rapidly than a sugar cube into tea. Gold, for example, is one of the most striking cases of the nanoscale boosting a material's reactivity. At less than 5 nanometers the typically inert substance becomes a catalyst that speeds up chemical reactions. Some chemists are leveraging the exaggerated surface area of gold nanoparticles to study potential cancer treatments where the particles carry therapeutic surface coatings and precisely attack tumors. Similarly, Iyer is collaborating with Los Alamos materials scientist Jennifer Hollingsworth to study how to adapt semiconducting nanoparticles called quantum dots for cancer therapy.



Unfortunately, the properties that make nanoscale materials valuable for biomedicine, or building the next generation of energy technologies, could come with a cost. Some nanoscale materials are more reactive with the body's proteins and DNA than their larger counterparts. If those risks go unrecognized, they could cause harm to human health, beginning at the cellular level.

A 2008 U.K. study was one of the first to address nanotoxicity in animals by investigating nanomaterials with a striking physical resemblance to asbestos. When researchers exposed laboratory mice to long, narrow carbon nanotube fibers, the mice developed tissue inflammation very similar to asbestosis—a chronic lung disease caused by asbestos. Curly or short nanotubes did not cause the same response, showing that nanoparticle toxicity can depend on properties like shape and size even when the chemical composition is the same.

Mentioning asbestos and nanoparticles in the same breath generates controversy, as some nanotechnologists warn that unwarranted panic over toxicity could stifle innovation. While there are no federal regulations specific to nanomaterials, Los Alamos and the Department of Energy have developed their own safety guidelines for worker and environmental protection (see "Nanosafety Starts Here," at right). Considering the breadth of nanotechnology research at Los Alamos, Iyer saw an opportunity to proactively understand nanotoxicology in parallel with the rapid discovery of new materials. "We're going to make these materials to address 21st century needs, like energy sustainability, but we need to understand their impact," she says.



Carbon nanotube

However, safer design won't happen by individually screening every single nanomaterial invented. Consider, for example, the variety of lengths, surface coatings, and manufacturing impurities for just the major kinds of single-walled carbon nanotubes (double-walled varieties also exist), and it's possible to generate more than 50,000 distinct samples just within that one category of nanomaterial. Toxicologists like Iyer could spend the rest of their lives doing nothing but testing nanotubes and hardly make a dent in the problem.

The dizzying array of nanoparticle features and the variety of ways researchers test their toxicity—from injecting live mice to exposing human cell cultures—is limiting how findings from researchers can aid industry or government agencies in developing nanomaterial safety policies. Testing each new nanostructure or its properties one at a time to identify the next asbestos amounts to looking for a nano-sized needle—or tube or wire—in a haystack. Iyer wants to streamline the haphazard nature of nanoparticle testing while developing guiding principles for materials scientists as they design and commercialize new particles.

She and others on her team are studying traditional toxicological responses like how particles affect cell growth, division, death, and metabolism. But they

nanosafety starts here

Los Alamos has been involved in nanotechnology research since the discipline's infancy. In 2006, the Center for Integrated Nanotechnologies (CINT) opened as part of the National Nanotechnology Initiative. Researchers from many institutions use joint CINT facilities at Los Alamos and Sandia National Laboratories to investigate all aspects of nanoscience and nanotechnology.

Part of the Los Alamos research is studying the toxicity of nanomaterials, while managing uncertainties about their risks to protect employees and the public. There are currently no state or federal regulations specifically addressing nanomaterials and no established recommendations for nanomaterial exposure levels. However, the National Institute for Occupational Safety and Health (NIOSH) and the Environmental Protection Agency also study nanotoxicity and provide safety recommendations.

The Department of Energy also created a formal order to provide guidelines for working with nanomaterials. Researchers and industrial hygiene professionals at Los Alamos and Sandia contributed, and the order is the foundation for nanomaterial safety policy at Los Alamos.

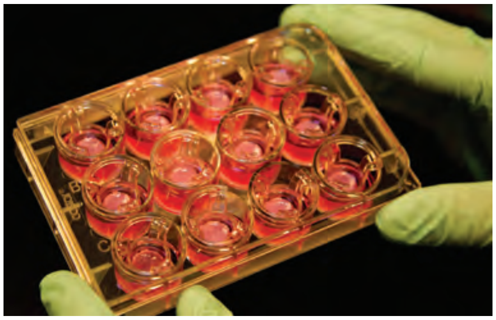
According to CINT Director David Morris, Los Alamos assumes that nanomaterials are at least as toxic as the bulk materials from which they are engineered. The Lab also recognizes that nanoparticles are potentially more toxic than the substances from which they are made. Understanding and predicting the extent of that toxicity is a major motivation for the collaboration between toxicologist Rashi Iyer and CINT scientist Jennifer Hollingsworth.

"No one appreciated that asbestos has toxicity above and beyond what the chemical constituents were until people started getting sick," says Morris. The Laboratory applies that lesson by minimizing researcher exposure to nanomaterials and keeping nanoparticles out of the environment.

For example, nanomaterial researchers at the Lab follow NIOSH recommendations and Los Alamos policies. Any potentially unbound nanomaterials, such as powders, in her lab are confined to chemical fume hoods or gloveboxes and stored in secure containers. The laboratory treats nanomaterial wastes as hazardous; they can't simply be poured down the drain.

"All the protections we have in place for working with carcinogenic or toxic chemicals are applied to nanomaterials," says Hollingsworth.

Los Alamos researchers work with very small nanomaterial quantities and take precautions while doing so. Their greatest concern is what happens when nanoparticles are made by the ton in industrial settings or in forms that could be inhaled. This is something the Los Alamos research aims to answer.



Human tissues for testing nanotoxicity are grown in quarter-sized wells that allow for rapid laboratory analysis.

are also finding early success with a new approach to the problem that drills down to the molecular level and explains how specific biomolecules within the cells of a tissue respond to nanoparticles.

A More Human Surrogate

Iyer and her colleagues learned that the field needed a more systematic approach when they observed in a 2010 study that even a small design tweak could influence a nanoparticle's toxicity. They exposed human skin and lung cells to molecules of buckminsterfullerene, a soccer ball-shaped cage of 60 carbon atoms configured like the geodesic domes of its namesake. Buckyballs, as they are sometimes called, are already manufactured in multi-ton quantities for use in sporting goods, such as lightweight tennis and badminton rackets, and are being tested as tiny vehicles for drug delivery.

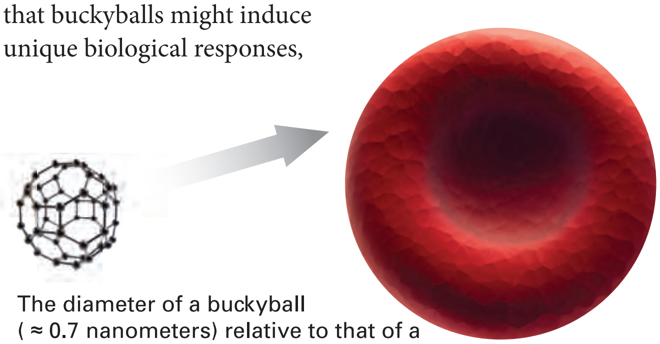
Iyer's chemistry colleague Hsing-Lin Wang selected three different buckyball variations: the standard pure carbon version and two with side chains—molecular adornments that are commonly attached to nanoparticles to change their behavior or function. When they exposed human skin cells to the buckyballs in the laboratory, one of the side chain varieties put cells in a kind of suspended animation. This process of senescence, where cells neither die nor divide, could cause organ dysfunction and eventually disease, but could also prevent cancerous tumors from expanding if scientists learn how to harness the effect.

The study was the first to find evidence that buckyballs might induce unique biological responses, including cellular aging. It also served as an important baseline for Iyer and her colleagues to learn how more complex tissues differ from single-cell layers when exposed to nanoparticles. Using single cell layers to mimic human exposure to a potential toxin, as in the buckyball study, is a common method in toxicology, but it's literally a one-dimensional approach. Monolayer cell cultures enable rapid testing but are a poor substitute for the diversity of interacting cells and chemical signals in real tissues and organs. For example, single-cell layers are immersed in liquid, but, as Iyer puts it, "we're not fish." Our own lung and skin tissues contact air on one side and fluid on the other, forming many cell types with defenses adapted for putting up a more concerted fight against invading nanostructures.

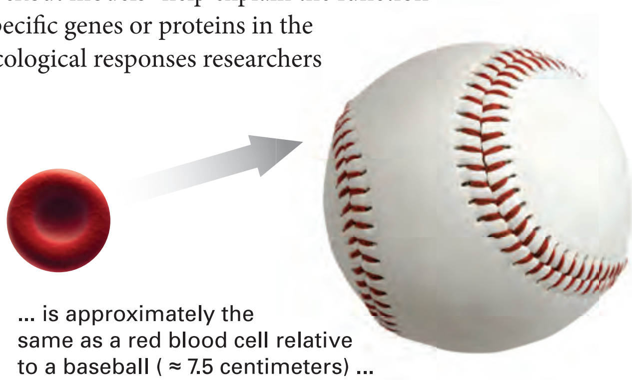
In addition to cell monolayers, non-human mammals like rats and mice are also common stand-ins for human testing. However, exposing them to nanoparticles is not just fraught with ethical dilemmas: their relevance to human toxicology is questionable, and their value is limited by the slow pace and expense of animal testing. A majority of the common chemicals we are exposed to daily have never been tested in animals. It's just not feasible, says Iyer. As animal welfare guidelines are beginning to encourage reduced animal use in research, animal testing's prominence in toxicology may wane.

For Iyer's team, a better mimic for exposure to nanoparticles is human lung and skin tissue constructed in the laboratory. Amber Nagy, a postdoctoral researcher in toxicology, came to Los Alamos specifically to work with Iyer to develop *in vitro* human lung tissue, which exists in a small dish outside of a human body.

While it is possible to order commercial lung tissue, making synthetic lung tissue is less expensive—less than 1/25th the cost—and gives the team more control over their experiments. The reduced expense alone is a compelling reason to develop in-house tissues, but there are significant scientific advantages as well. For example, commercial tissues can't be readily manipulated, while Iyer's group can use their own inventions to delete a particular gene or protein. These "knockout models" help explain the function of specific genes or proteins in the toxicological responses researchers



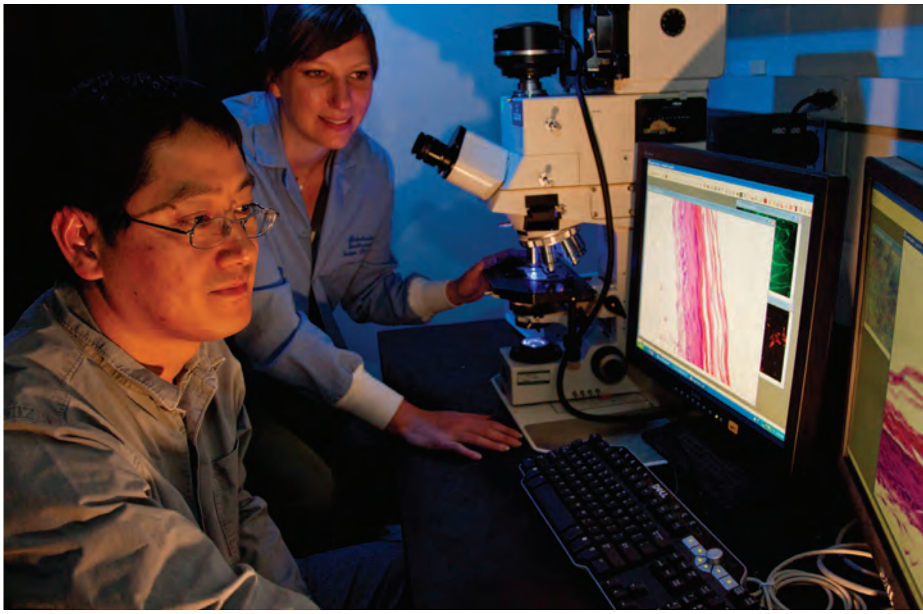
The diameter of a buckyball (≈ 0.7 nanometers) relative to that of a human red blood cell (≈ 8 micrometers) ...



... is approximately the same as a red blood cell relative to a baseball (≈ 7.5 centimeters) ...

observe and would complement Iyer's systematic approach for predicting how individuals will handle nanoparticle exposure.

Los Alamos toxicologist Jun Gao joined Iyer's nanotoxicity team in 2007 and has successfully grown a multi-layer human skin tissue, which Gao and Iyer are finding considerably more realistic than a traditional cell monolayer. If Iyer and her team learn how to control key variables, such as skin pigment expression or cell involvement in allergic responses, they could eventually perform human population studies in the laboratory without ever exposing people to potential toxins. Custom-grown tissues could eventually let them test how smokers and non-smokers or people with different ultraviolet exposure histories and skin pigments will respond to different nanoparticles.



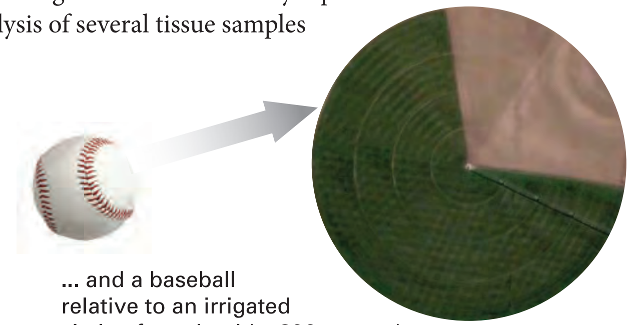
Los Alamos researchers Jun Gao (left) and Amber Nagy examine the lab-grown tissues they develop.

Developing human tissue in a tiny dish is more than simply creating a layer cake-like mixture of different cell types. Gao and Nagy must confirm that they have grown something that behaves like human tissue. To validate the function of their engineered human lung tissues, they turn to asbestos, a well-known lung toxin with decades of research explaining how it damages tissue. When exposed to crocidolite asbestos, one of the more hazardous varieties of the mineral, both natural and artificial tissues respond with inflammation, a decrease in mitochondrial metabolism, and a specific type of cell death. The tissues must also be the same down to the molecular level, or the resemblances are only superficial. Morphological markers such as gel-forming proteins called mucin, hair-like cell extensions called cilia, and tight junctions between cells, tell Nagy and Gao that they've made a genuine tissue mimic, not just a soup of cells in a tray.

Getting Charged Up

With tissues constructed, Iyer and her team are now working to predict which nanoparticles will be toxic and which will be harmless. Using cutting-edge technologies that allow for very rapid analysis of several tissue samples at once, they are able to monitor changes in protein- and gene-level characteristics of the nanomaterial. These "omic" technologies are coming to the forefront as ways to measure impacts on the entire collection of genes (the genome), proteins (the proteome), metabolites (the metabalome), or RNA (the transcriptome). With each particle they test on each cell type, Iyer's proteomics team, Srinivas Iyer and Tim Sanchez, generates data on how gene and protein regulation changes depend on a particular nanoparticle or its properties.

To analyze the gene transcription and protein expression data that could be linked to toxicity, they turn to Los Alamos computational biology colleagues Jeffrey Drocco and Jian Song. By using statistical tools to look at the data in a mathematically unbiased way, Drocco and Song find otherwise hidden relationships between toxicity and molecular responses. In the near future, understanding those relationships could enable the discovery and identification of nanomaterial-specific biomarkers to develop diagnostic tools that will determine past and current exposure to nanomaterials.



... and a baseball relative to an irrigated circle of cropland (≈ 800 meters).

Buckminsterfullerene ("buckyball"), a spherical nanoparticle with 60 carbon atoms, is less than one nanometer in size—insidiously small relative to the cells of the human body. It's roughly 10,000 times smaller than a red blood cell, which is comparable to the difference between a baseball and an irrigated circle of cropland that's easily visible from an airplane.

If Iyer and her team learn how to control key variables ... they could eventually perform human population studies in the laboratory ***without ever exposing people to potential toxins.***

The approach has yielded results that the toxicologists would have missed on their own. Through statistical sleuthing, Song found that when Iyer's team exposed skin cells to fullerenes, the genes perturbed were associated with heart toxicity. "You don't really have to use heart cells to figure out if something is a heart toxicant," says Iyer. "Down the line, the idea is that if you have 10,000 nanomaterials and you look at the molecular level response you should be able to *predict* toxicity."

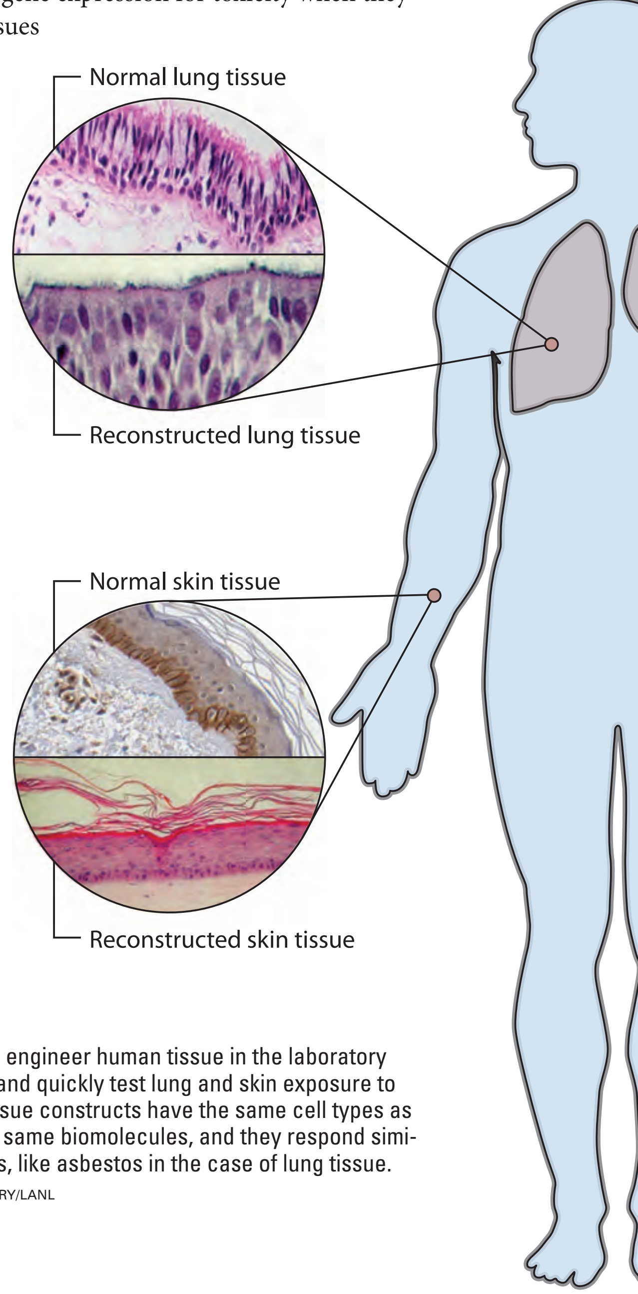
Iyer and her team first tested their molecular approach in a pilot study published last year. They exposed human lung cells to semiconducting nanocrystals engineered by Jennifer Hollingsworth, who designs materials for energy efficiency and biomedical applications as part of Los Alamos National Laboratory's Center for Integrative Nanotechnologies. Called quantum dots, the particles have optical and electronic properties that can be fine-tuned by changing their size, making them promising light emitters in energy-efficient LED lighting. Their size-dependent fluorescent colors are also ideal for staining and imaging live cells in exquisite detail and have potential application for detecting and treating cancer.

Much like radiation used in cancer treatment, quantum dots could be life-saving but could cause harm through unplanned exposure. As quantum dots are mass-produced for applications like LEDs, solar cells, and medicine, Hollingsworth wants to help bring toxicological knowledge into her designs. "I'm involved because I want to design materials that will either have a minimal biological impact or a predictable one," she says.

Iyer's group is already making some generalizations that could help Hollingsworth with that goal. When they used a variety of quantum dots to treat a single layer of cells that line the lung's bronchia, they found that positively charged dots were much more deadly to cells than their negatively charged counterparts, regardless of the length of side chains attached to the dots or their overall size. In fact, these materials perturbed distinct suites of genes, proteins, and pathways that might be due to the specific charge on the nanomaterial surface. The team has learned that negatively charged quantum dots and those with short side chains were the least toxic and could be the best option for medical applications. However, even in quantum dots that appear benign by traditional measures of toxicity, molecular-level data revealed that they increase gene expression associated with DNA damage.

The toxicity of positively charged nanoparticles isn't simply an aberration of quantum dots. Through their molecular data, the team sees a correlation between positive particle charge and gene expression for toxicity when they expose cells and tissues of lung and skin to many kinds of nanomaterials, including carbon nanotubes and buckyballs. When Drocco analyzes the data, the team notices that positively charged particles disrupt transcription, the first step of gene expression.

"It's not by chance," says Nagy. "We're able to separate the signal from the noise and see that there's a clear transcriptional response induced by nanomaterials of different charges. We don't



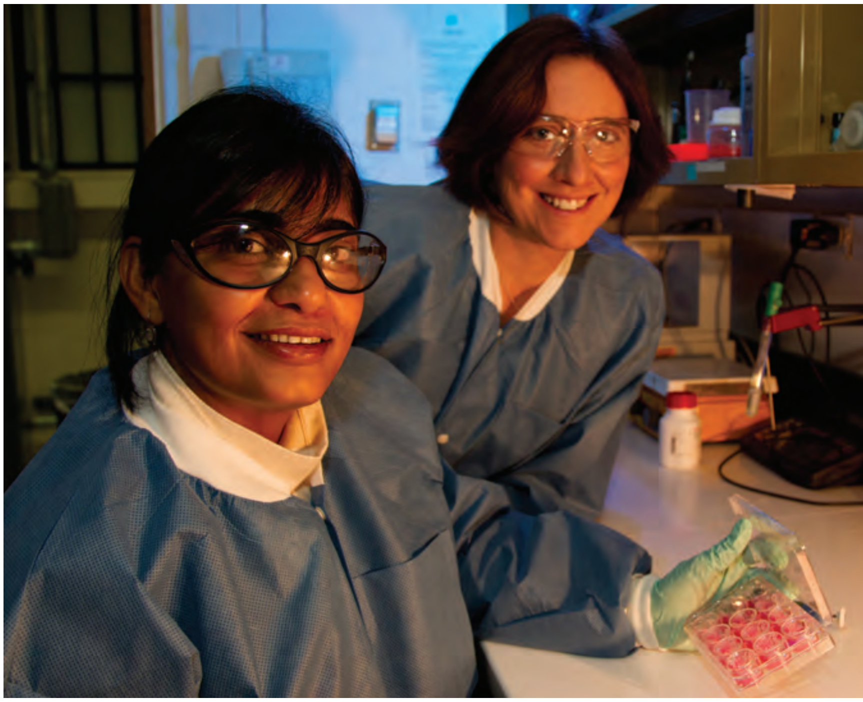
Los Alamos scientists engineer human tissue in the laboratory to realistically mimic and quickly test lung and skin exposure to nanoparticles. The tissue constructs have the same cell types as human tissue and the same biomolecules, and they respond similarly to known irritants, like asbestos in the case of lung tissue.
CREDIT: RASHI IYER LABORATORY/LANL

want a positively charged anything—unless we are trying to kill the cell—because it seems to induce more perturbation."

When the team exposes lung and skin tissues to nanoparticles, they see patterns of toxicity that mirror single cell layers treated with nanoparticles. Charge, side chain selection, and particle size are all factors in harming both cells and tissues. But with tissues, the cellular and molecular responses are much less severe (or even nonexistent) than those for the same dose applied to cells.

In lung tissues, protective mucous and tiny waving arms called cilia trap invading particles and move them away from the tissue, but those defenses are absent in single cell layers. "We've found that once you add structural complexity and different cell types, the biological response we observe is actually from all those different cell types in the tissue, not just the one type of cell," says Gao.

They're also using the complexity of tissue constructs to learn which nanoparticles are most likely to move through skin and circulate to other organs. Gao is imaging particles as they've lodged in different layers of skin. For example, he found that negatively charged quantum dots penetrate skin tissue while positively charged dots sever the tissue without much penetration. The results will assist with nanomaterial design for targeted drug delivery and determine which particles completely pass through several layers of human skin tissue.



Toxicologist Rashi Iyer (left) and materials scientist Jennifer Hollingsworth collaborate to predict and mitigate the toxicity of nanoparticles before they are mass produced.

Bringing *In Vitro* to Life

While toxicologists can't experiment with how a real human body responds to rogue nanoparticles or those used for medical purposes, Iyer is leading an effort to build the next best thing—a laboratory device that simulates human physiology and chemistry at 1/1000th the scale of a human body. This system of engineered human organs—the Advanced Tissue-engineered Human Ectypal Network Analyzer (ATHENA), as it is named—will rapidly screen for the safety of nanoparticles and pharmaceuticals without the need of animal exposure studies. Moreover, Iyer and her colleagues are working toward developing ATHENA to study human exposure to biological weapons and test possible medical countermeasures.

In addition to overseeing the unification of an artificial heart, lung, liver, kidney, and arterial and venous systems with artificial blood, Iyer's group will breathe life into ATHENA by mimicking the bronchial and alveolar architecture of the human lung. The idea is to develop a platform that enables organ-to-organ communication to simulate the human body's response to any pathogen, material, drug, or chemical. Then, to take into account the physiological responses of organs that are not represented in ATHENA, Iyer has added placeholders for missing organs that will simulate the organ of choice, depending upon the nature of the investigation. "This is really the first time that a system of such magnitude and complexity will be developed, with the potential to eventually replace animal and human clinical studies," says Iyer.

Iyer isn't alone in her ambition to someday replace animal studies with technology that simulates our relationship with the materials we invent. The National Institutes of Health and the Defense Advanced Research Projects Agency are behind similar "human-on a-chip" technologies, funding separate teams to develop the next generation of bioassessment platforms. "It's a race to build a good version of Frankenstein's monster," she says, quickly adding that her engineered human will benefit society in a way the fictional one never could. ❖ LDRD

—Sarah Keller

Laid to Rest

The Laboratory is cleaning house

and sending decades' worth of nuclear waste to a salt-encrusted grave.

THE BIG 18-WHEELER with its strange-looking cargo trailer rumbles down Pajarito Road and straight through the heart of Los Alamos National Laboratory's 36-square-mile campus, passing perhaps a half dozen technical areas, a few variegated meadows, and some pristine high-desert terrain before intersecting New Mexico Route 4, which serves as the Laboratory's eastern boundary. The truck's specialized trailer is one of several used by the Department of Energy (DOE) to transport transuranic nuclear waste, also known as TRU waste. Such waste consists of items, for example, lab coats and lab equipment, that have been contaminated with any of the radioactive elements heavier than uranium: primarily plutonium, neptunium, and americium. The loaded truck makes a left and continues its scheduled run to the Waste Isolation Pilot Plant (WIPP), some 300 miles distant in southeastern New Mexico.

WIPP is the nation's only licensed deep geologic repository for nuclear waste. When the truck arrives, its radioactive cargo will be inspected, loaded onto an elevator, and ferried 2150 feet underground, where a huge warren of tunnels and cavernous catacombs has been hogged out from the middle of a half-mile-deep bed of natural salt. The waste packages will be moved into an available room, set in place, and unceremoniously laid to rest.

It seems straightforward—gather waste, bury it underground—but this is a challenging business, disposing of TRU waste. Every step needs to be done correctly, or small problems can quickly become big ones. The route taken by the WIPP truck, for example, goes around Santa Fe (the state capital), through Roswell (the state's extraterrestrial capital), through numerous small western towns, and crosses miles of culturally and environmentally sensitive land. Any incident that would expose the public to even a minor amount of radiation would have major consequences.

Kathryn Johns-Hughes oversees the Laboratory's TRU Program, which as per agreement between the New Mexico State Environment Department (NMED) and the Department of Energy (DOE), aims to ship a total of 3706 cubic meters of accumulated TRU waste to WIPP by June 2014. It's a demanding goal. Unofficially, about 650 shipments will be needed to move that much material, a number that's on par with the total number of shipments made in the first 12 years that Los Alamos has been shipping waste to the repository.

But Johns-Hughes works with a world-class team of overachievers. They found ways to process the waste more efficiently, and the results have been remarkable.

"Our goal for the 2012 fiscal year was to make 184 shipments to WIPP," Johns-Hughes said. "We easily exceeded that and made 230, and we plan to make on the order of 300 shipments this fiscal year."

The accelerated pace was achieved without cutting corners or compromising safety or security, a priority that has been paramount since day one of operations. Indeed, in more than 1100 trips to WIPP, no truck has ever failed to reach its destination. There have been no accidents, no spills, no release of radiation of any kind.

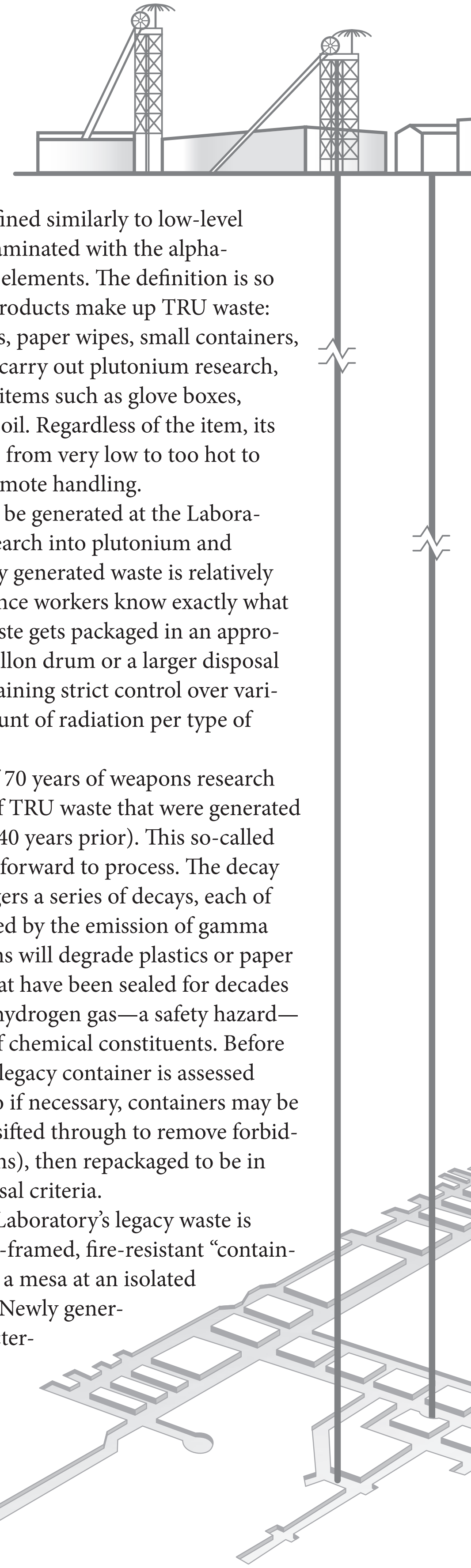
Transuranic (TRU) waste can be any item that has been contaminated with alpha-particle-emitting elements heavier than uranium—primarily plutonium, but also neptunium, americium, and curium. TRU waste is transported by truck to WIPP. The supersized steel containers on the truck bed are nearly indestructible, each capable of carrying 14 fifty-five-gallon steel drums of TRU waste.

"It's largely due to a strict adherence to procedures and a team that takes pride in its work," said Johns-Hughes about the sterling track record. "We ship nuclear waste. It's not a glamorous project, but it's a worthwhile one. We're proud to help Los Alamos clean up the past and have a sustainable future."

TRU Waste

The United States categorizes nuclear waste according to process, not level of radioactivity or hazard potential. High-level nuclear waste, for example, is fuel that has either been irradiated in a nuclear reactor or material generated from the reprocessing of that fuel. It consists of unfissioned uranium fuel, transuranic elements that were created from the uranium, and highly radioactive fission products. Low-level nuclear waste consists of items that have been contaminated as a result of exposure to radiation.

Los Alamos stores much of its TRU waste at an isolated site known as Area G. (Top) The long white structures are containment domes—metal framed, fire-resistant warehouses. (Bottom) About 20 percent of the Laboratory's TRU waste is packaged in steel barrels, awaiting transport to WIPP.



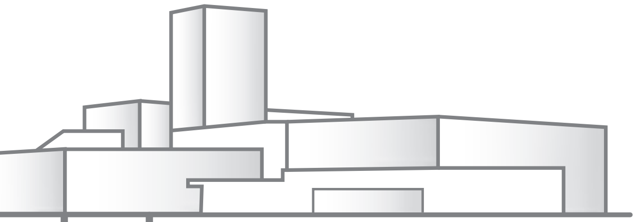
Transuranic waste is defined similarly to low-level waste, it being anything contaminated with the alpha-particle-emitting transuranic elements. The definition is so broad that a huge variety of products make up TRU waste: used protective clothing, tools, paper wipes, small containers, the various whatnots used to carry out plutonium research, as well as large and unwieldy items such as glove boxes, machinery, or even layers of soil. Regardless of the item, its radioactive content can range from very low to too hot to handle, the latter requiring remote handling.

TRU waste continues to be generated at the Laboratory as a result of current research into plutonium and other transuranics. This newly generated waste is relatively straightforward to process, since workers know exactly what they are dealing with. The waste gets packaged in an appropriate container—say, a 55-gallon drum or a larger disposal container—with crews maintaining strict control over various limits, including the amount of radiation per type of storage container.

But part of the legacy of 70 years of weapons research and development are stores of TRU waste that were generated prior to 1994 (some of it like 40 years prior). This so-called legacy waste is not so straightforward to process. The decay of a transuranic element triggers a series of decays, each of which is typically accompanied by the emission of gamma rays. The decays and emissions will degrade plastics or paper goods, so waste containers that have been sealed for decades frequently have a buildup of hydrogen gas—a safety hazard—or an unknown breakdown of chemical constituents. Before being shipped to WIPP, each legacy container is assessed and, if necessary, vented. Also if necessary, containers may be opened, the waste extracted, sifted through to remove forbidden items (such as aerosol cans), then repackaged to be in compliance with WIPP disposal criteria.

At present, most of the Laboratory's legacy waste is stored in aboveground, metal-framed, fire-resistant "containment domes" that reside atop a mesa at an isolated LANL site known as Area G. Newly generated TRU waste is also characterized and stored at Area G. In 2011, the Las Conchas wildfire burned more than 156,000 acres of the Jemez Mountains surrounding Los Alamos and

WIPP is the nation's only licensed underground nuclear waste repository. It accepts only defense-related TRU waste. The storage caverns lie some 2150 feet below the surface, carved out of an enormous bed of salt.



came within 3.5 miles of Area G. It prompted the framework agreement between the DOE and NMED that resulted in Kathryn Johns-Hughes' dedicated team working very hard to remove 3706 cubic meters of TRU waste. Ultimately, the Laboratory plans to close Area G and to transfer TRU waste management capabilities to the to-be-built TRU Waste Facility. (See "Intelligent Design" on page 15.)

None of this happens unless WIPP is happening, so to speak, which it is, much to the delight of a Carlsbad community that has voiced strong public support for the repository. After 13 years of operations, WIPP has demonstrated an impressive fiscal and operational efficiency. And it all shakes out because of salt.

Any item contaminated with trace amounts of a transuranic element can be classified as TRU waste. This x-ray image, taken of a TRU waste storage container, reveals pipes and a sprinkler head from a discarded fire safety system.

WIPP and the Miracle of Salt

WIPP is carved out of an enormous layer of common salt (sodium chloride, NaCl) that formed when an inland sea evaporated approximately 250 million years ago. Termed bedded salt, (as opposed to domal salt, which is shaped like an enormous underground mushroom), it runs for hundreds of miles, from southern Texas and southeast New Mexico, through the Texas panhandle and all the way up to Colorado and Kansas. Such formations are common throughout the United States and the world and have been mined for millennia for table salt. Engineers have been able to tap into a wealth of information on how to mine salt efficiently and what to expect for WIPP's system of tunnels and rooms.

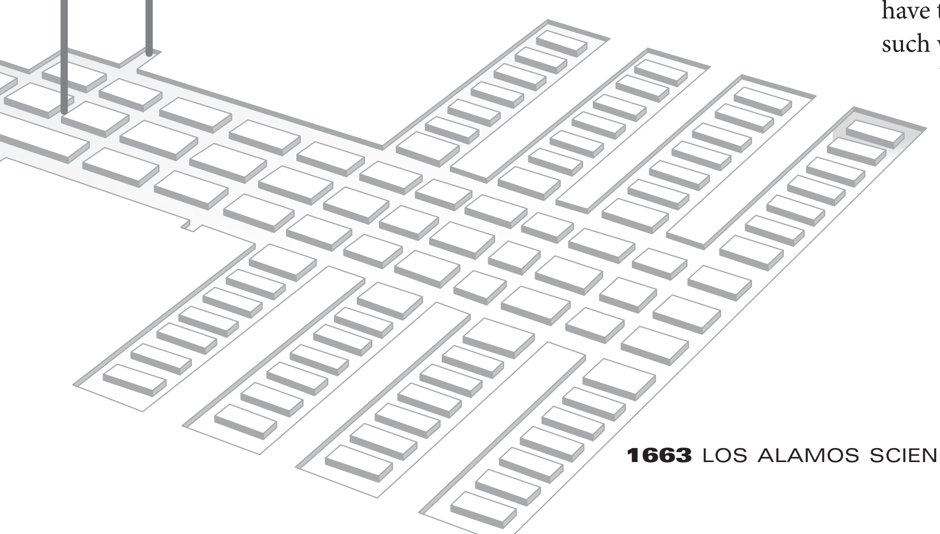
Given that the bedded salt formation has remained intact for hundreds of millions of years, the expectation is that it will continue to remain intact for many million more. That's good news for a repository that is intended to keep its radioactive contents isolated for millenia. Furthermore, the salt formation's existence is an indication that water is unable to penetrate into the undisturbed salt. Water is an overriding concern for a repository; it can corrode a waste container, dissolve the contents, and transport the radioactive material off site. But the salt's permeability to water is evidently low, or else much of the bedded salt would have dissolved over time. Its permeability is so low as to be unmeasurable using traditional hydrological and reservoir engineering methods.

Still, the property that makes salt a particularly favorable waste disposal medium is its ability to creep, or flow slowly. This unique mechanical behavior occurs in response to the pressure exerted by the rock overburden. One consequence is that fractures that open in the salt due to mining operations or earthquakes will, over time, heal as the salt creeps into the open space, and any cracks or fissures that could have served as conduits for water to enter the repository get sealed shut. The other consequence is that over time the salt should creep and flow around an emplaced waste container, sealing it in a waterproof, timeless tomb.

Hot Solution

WIPP's salt *is* creeping, as expected. It raises the possibility that a new repository carved out of bedded salt could serve as a disposal medium for materials that are prohibited from being buried at WIPP: namely, defense-related, high-level nuclear waste and spent fuel from commercial nuclear power plants. Of course, any new salt repository would have to be approved and licensed before it could accept such waste.

Ned Elkins is the Laboratory's Repository Science and Operations group leader. Stationed in Carlsbad, New Mexico, near the WIPP site, the group provides technical support to the DOE's Office of



Depending on the impurities embedded within it, the salt from WIPP can be anything from a reddish, relatively opaque rock to a clear crystal like the one shown here.

Environmental Management for nuclear issues and advises other institutions on how to technically achieve their goals, consistent with DOE objectives. Members of the group have already provided information to the DOE on the feasibility of a high-level nuclear waste repository in a subterranean bedded salt formation.

"High-level nuclear waste gives off substantial heat," said Elkins, "so you would have a heat source (the waste) sealed inside a waste package, surrounded by other hot waste packages, and they're all getting slowly enveloped by salt. Not surprisingly, there's little data about the integrated mechanical, hydrological, and chemical behavior of that system."

What is known is that salt is an excellent thermal conductor, and it's ability to conduct heat away from a source is approximately three to five times higher than other potential geologic media, such as crystalline rock or clay. This is a positive attribute, as the heat would be rapidly dissipated into the surrounding formation. A series of laboratory-scale experiments and a modeling effort has been proposed that will investigate the behavior of salt under high-heat conditions.

Elkins, however, argues that no amount of laboratory testing or modeling alone would be adequate to prove the performance of a nuclear waste repository, and that field tests should be an essential part of any licensing program. Field tests to investigate the properties of hot salt are planned and would take place in a remote part of WIPP known as the Salt Disposal Investigations Research Area, consisting of more than 8000 linear feet of newly excavated tunnels.

It's expected that the creep rate will increase with temperature, so the waste will get encased faster; but at very high temperatures, the salt may actually burst as tiny pockets of water trapped within the salt vaporize and expand. The results of both the laboratory and field experiments will be used to improve predictive models of the thermo-mechanical-hydrological behavior of the hot salt so that any future repository site can be expertly evaluated.

Whether a new repository will be built or not will be debated at the national, state, and local levels. In the meantime, WIPP will quietly go about its business, receiving shipment after shipment of TRU waste. It is, to date, a successful experiment in the proper disposition of nuclear waste and helps do what everyone wants to do: clean up, protect the public, and be responsible.

—Jay Schecker

Rocky Flats, the Cold War-era complex that manufactured plutonium triggers for nuclear weapons, was shut down in 1989 because its facilities, soil, and groundwater had become seriously contaminated with plutonium. More than 800 buildings were decontaminated and demolished, and the contaminated concrete was shipped to WIPP. Remediation of the soil, initially thought to be a monumental problem, was found to be tractable after a Los Alamos-led scientific team determined that the plutonium in the soil had formed hydrated plutonium dioxides, which adhere to soil particles. The information led to a much better understanding of how to remediate the site, namely by removing just the top 10–12 centimeters of soil. The soil remediation effort finished a year ahead of schedule, with a likely cost savings of billions of dollars.

Intelligent Design

Dan Vitaletti, TRU Waste Facility Design Manager, is clearly excited as he talks about the to-be-built TRU Waste Facility (TWF). Slated to open in 2015, the new facility will be part of a comprehensive, long-term strategy to consolidate hazardous and radioactive waste operations at the Laboratory into a smaller, more compact area. Currently, all TRU waste is stored and characterized at an isolated Laboratory site known as Area G, which has been used for waste disposal since 1957.

"We're going from 66 acres at Area G down to six acres," Vitaletti says, "but the facility will have superb capability to manage all newly generated TRU waste."

Vitaletti asks Brad Pulliam, design engineer, to bring up a drawing of the TWF on a computer. Instantly, the monitor displays a detailed, 3-D rendering of the facility, one of the many benefits of using Building Information Modeling (BIM) software to design the facility. The BIM software melds the tools of computer-aided design (CAD) with a powerful database. Anything having to do with the facility—blueprints, work orders, inventory lists, maintenance schedules—becomes integrated into an all-encompassing project model. It allows designers, contractors, and users alike to check out every aspect of the facility, from the layout of the ventilation system to the serial numbers of the supply closet keys.

Pulliam shifts the point-of-view and focuses on a large, warehouse-like building.

"Waste containers will be stored in enclosed buildings before they're shipped to WIPP," says Vitaletti. "We'll also validate and certify the containers for shipment."

"Now let's talk protection," he says, and he delves into describing several of the facility's enhanced protection features. Federal law requires that almost any type of potential hazard, accident, or possible insult to the facility be analyzed and controls to mitigate such insults be approved by the DOE. The Defense Nuclear Facility Safety Board and other governmental or independent entities scrutinize the entire safety analysis.

"The design of this facility was driven by the accident safety analysis," says Vitaletti. "For example, we needed to have roadside barriers that were strong enough to stop a large vehicle from entering the site. Currently, the TWF's barriers are designed to stop a 10,000-lb truck moving at 50 miles per hour, but we're looking to upgrade to a barrier that will stop a similarly moving 65,000-lb truck."

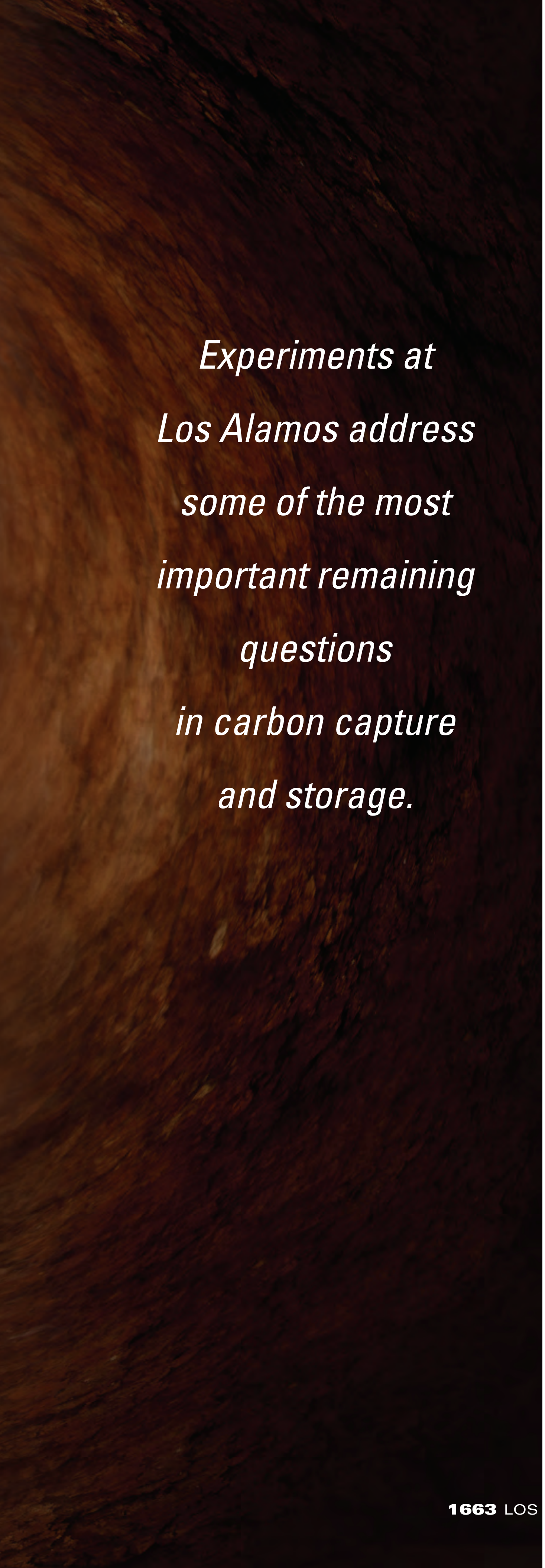
He continues: "The facility is protected by a seismic switch that will cut power in case of a seismic event, and by a dedicated fire suppression system in case of a fire. There's a minimum of 75 feet of clear space around the facility that affords us protection against wildfires. We even changed sites to get farther away from the Los Alamos airport to minimize the risk an airplane crashing into the facility."

Really?

"We designed this to be an enduring facility that will operate safely, securely, and effectively for the foreseeable future," says Vitaletti. "So yeah, Really!"

PUTTING CARBON BACK where it came from

Most of the world's existing energy supply is stored underground in hydrocarbon fuels. The fuels are extracted and then burned, releasing carbon dioxide into the atmosphere and driving increasingly rapid climate change in the process. But a large-scale, international research program is working to overcome the remaining obstacles to putting that carbon back into the ground where it came from, and Los Alamos scientists are making significant progress on many fronts.



Experiments at Los Alamos address some of the most important remaining questions in carbon capture and storage.

ADAPTING TO CLIMATE CHANGE WILL BE COSTLY. Severe weather events such as Superstorm Sandy, for example, result in huge costs for cleanup and repairs, and these events are increasingly associated with global climate change. As the climate warms due to the rising buildup of greenhouse gases in the atmosphere—primarily carbon dioxide (CO_2)—powerful storms continue to rack up public expense. And while it is impossible to attribute any particular storm to climate change, the increasing frequency and severity of storms is a predicted consequence of it.

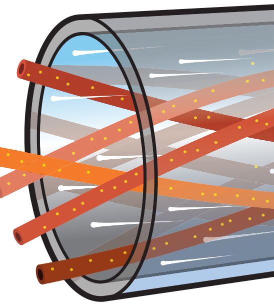
Yet severe storms are just the tip of the melting iceberg. Rainforest, coastal, and wetland ecosystems are all at risk, as are the benefits they provide in terms of natural resources (food, wood, medicine) and services (water filtration, runoff control, carbon sequestration). In addition, any shift in water availability may threaten more frequent and more extreme droughts in some areas coupled with frequent and extreme floods in others. Wildfires, crop failures, and famine are possibilities. So, too, are malnutrition, water-borne illness, and the spread of infectious disease. All of this represents a steep price to be paid in lives and dollars.

The primary human contribution to climate change is CO_2 emissions from fossil-fuel-based energy production. And for the foreseeable future, fossil fuels will remain the world's leading energy source because they are cheap and effective relative to renewables. Indeed, in the developing world, where the population increases are greatest, access to cheap energy is often considered critical to modernization. So mitigating the potential consequences of climate change depends on somehow reducing CO_2 output, yet the scale at which this must be done to offset human fossil fuel consumption is immense—posing a science and engineering challenge worthy of the national laboratories.

Deep Storage

Rajesh Pawar is the senior project leader of several Los Alamos partnerships working to test the feasibility of capturing most of the CO_2 produced by power plants and pumping it into geological storage reservoirs deep underground. Broadly referred to as carbon capture, utilization, and storage (CCUS), the effort aims to reduce the flow of CO_2 to the atmosphere. Pawar and his colleagues at Los Alamos, other national laboratories, and research sites around the world are working to create a commerically viable process in which, after the fossil fuels have been pulled out of the ground and consumed for energy, the residual carbon is properly put back where it came from.

Like any major energy-related undertaking—drilling for oil, burning coal, splitting atoms, or transmitting electricity—CCUS will involve some risk. Potential dangers include leaks and blowouts on the surface as well as groundwater impacts underground. These risks must be researched and understood in order to manage and minimize them in practice and develop technology to mitigate negative impacts. Safety and control systems must be designed, and the CCUS workforce must be trained to make sure the CO_2 stays where it belongs. That's why Pawar and others are busily investigating every facet of the problem before CCUS technology can be tested at a larger scale.



Although the nation's major initiative in CCUS has only been up and running in force for about 10 years, the oil and gas industry has been pumping pressurized CO_2 into underground oil reservoirs for enhanced oil recovery since the 1970s. The CO_2 acts to mobilize unrecovered oil, effectively making the oil easier to extract; this is, in fact, one type of utilization—the U in CCUS. Now, in order to reduce the amount of CO_2 entering the atmosphere, CCUS programs seek to pump supercritical CO_2—high-pressure, high-temperature CO_2 that expands to fill its container like a gas but can be pumped like a liquid—to a depth of more than a kilometer. The injected CO_2 will reside below drinking water aquifers in a porous rock layer. To take advantage of the same geological process that has long preserved oil and gas deposits in the subsurface, carbon storage reservoirs must have an impermeable caprock layer above the porous layer to prevent the buoyant CO_2 from migrating upward.

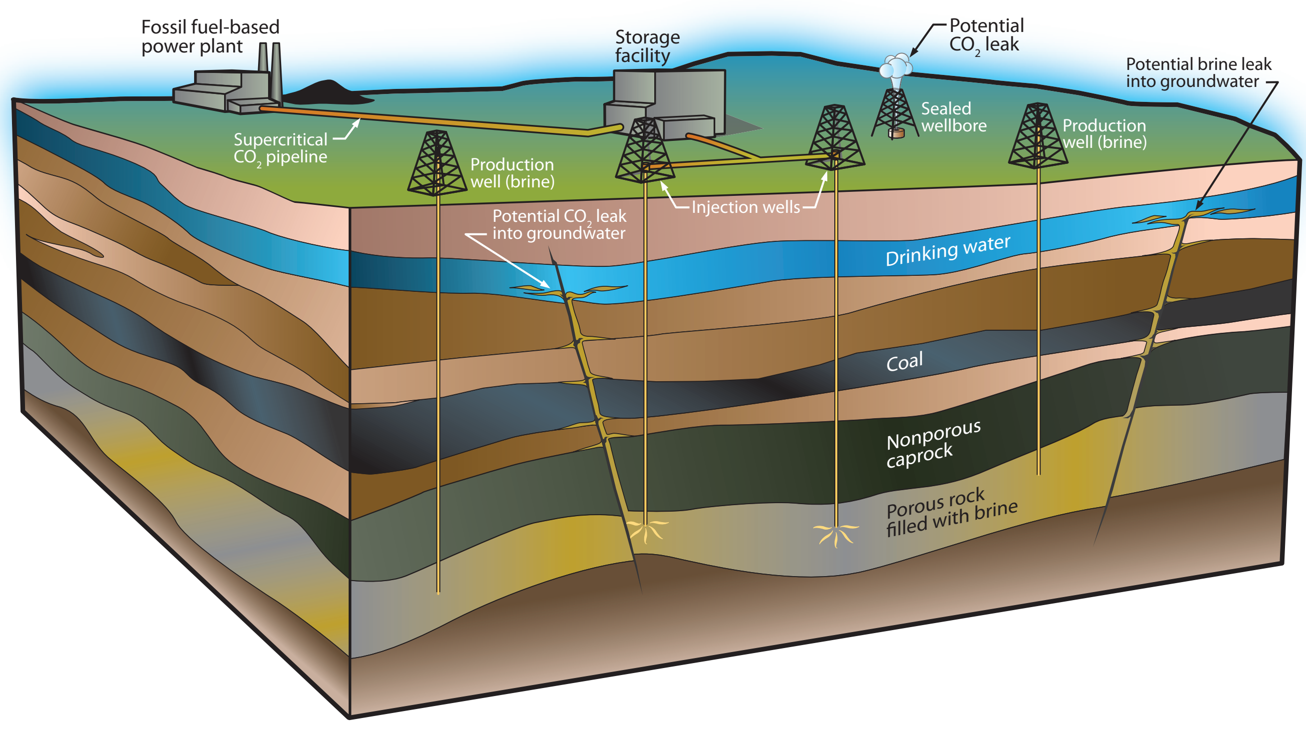
"One common misconception about carbon storage," says Pawar, "is that the underground storage reservoirs are empty, cavern-like structures. In fact, they consist of solid rock with tiny pores that are completely filled with salty, undrinkable water." Therefore, injected supercritical CO_2 must either displace the existing fluid—potentially requiring other deep wells to draw out the displaced salty water, called brine—or increase the subterranean pressure as more of the compressible, supercritical fluid is pumped into a finite space. In practice, both extracting brine and increasing pressure can occur in varying degrees. But because increased pressure poses challenges, including the potential to cause micro-earthquakes, the injection must be done with care. Fortunately, with time, some of the CO_2 will naturally dissolve into the brine, become trapped by capillary forces, or react with the rock, immobilizing the CO_2 and thereby reducing the pressure.

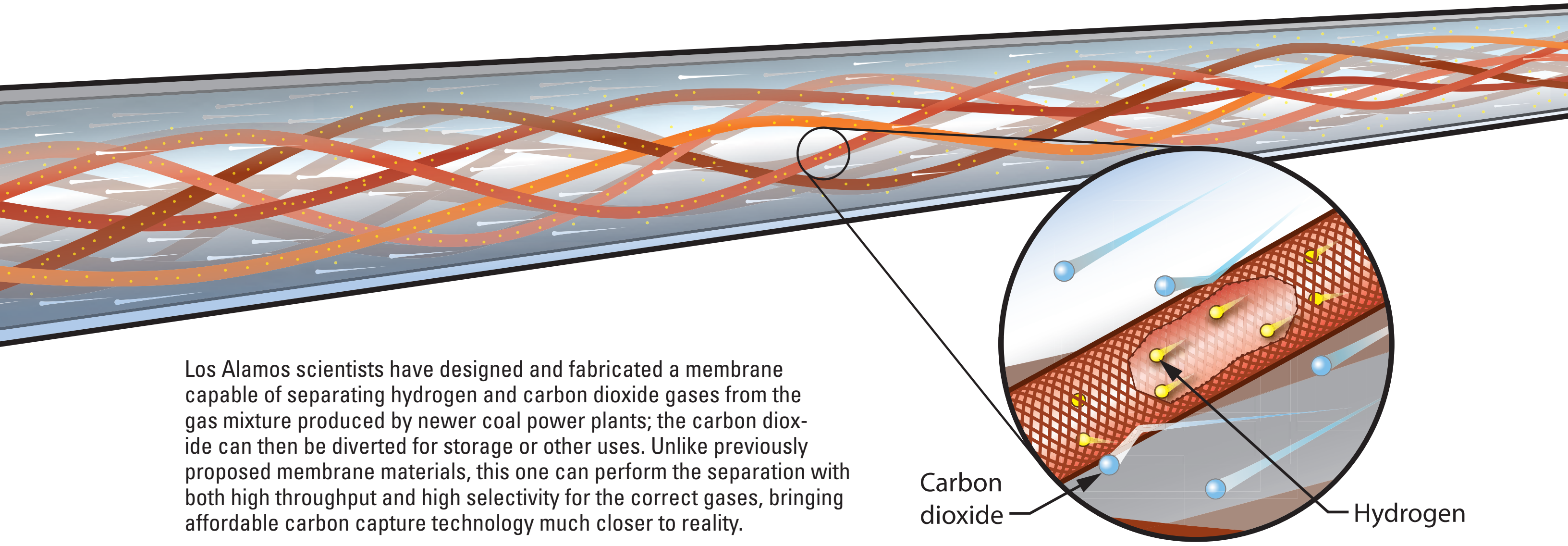
Infrastructure for CO_2 storage begins with a dedicated pipeline to transport supercritical CO_2 from the power plant, where the CO_2 must be captured, to the storage facility. There, injection wells (center) pump the CO_2 more than a kilometer underground to a porous rock layer containing salty water known as brine. Above this injection layer lies a wide, nonporous caprock layer to keep the CO_2 mixture in place in spite of its natural buoyancy—the same geological mechanism that keeps pressurized oil and gas reservoirs intact. To alleviate the pressure increase caused by the injection of CO_2, multiple production wells (left and right) may extract hot brine from the deep reservoir, providing a potential source of both geothermal energy and industrially usable water.

As with other large-scale energy applications, the carbon storage facility must be managed to prevent potential problems. In particular, its operators must continually monitor the field for evidence of CO_2 escaping from its storage reservoir. This can happen if defects in the rock layers create an upward migration path. Such defects can occur along geological faults (diagonal lines) or wellbores, and any migrating CO_2 might end up in two places of concern: drinking water reservoirs and the atmosphere. Similarly, brine might migrate along the same defect paths up to a drinking water layer, bringing with it salt and potentially harmful heavy metal contaminants.

Comprehensive monitoring to keep abreast of any such migration includes seismic imaging of the underground storage reservoir; direct sampling from key underground sites closer to the surface, including along well bores and in drinking water reservoirs; and sensor-based scanning across the surface for elevated CO_2 levels. Experience to date demonstrates that leaks to the surface are rare and can be detected early and corrected.

Los Alamos research has led to significant improvements to virtually every aspect of this complex, multifaceted effort: more efficient CO_2 capture at the power plant, better understanding of the potential for groundwater contamination by CO_2 or brine (including which sites are likely to avoid the problem and under what conditions it might naturally resolve itself), sealing off retired well bores such that any microscopic defects will exhibit self-healing, detecting evidence of stored CO_2 migration against a background of natural CO_2 sources, and analyzing potential storage sites for geological and economic suitability.





Los Alamos scientists have designed and fabricated a membrane capable of separating hydrogen and carbon dioxide gases from the gas mixture produced by newer coal power plants; the carbon dioxide can then be diverted for storage or other uses. Unlike previously proposed membrane materials, this one can perform the separation with both high throughput and high selectivity for the correct gases, bringing affordable carbon capture technology much closer to reality.

However, the ability to successfully manage underground storage depends not only on the quantity and pressure of the material to be stored, but also on the duration. Ideally, if the material could be stored for hundreds of thousands of years, it would have time for slow reactions with the surrounding rock that result in solid carbonate minerals, which could remain there indefinitely, unsupervised. But the technical challenge of ensuring such a long storage period borders on the impractical. On the other hand, if the storage period is too brief, the world won't have enough time to switch to alternative energy sources that don't produce CO_2. Experts and policy makers have, therefore, decided to target an intermediate time scale of approximately 1000 years. As the thinking goes, if the stored CO_2 leaks slowly over this time period, it won't be terribly damaging because the world will be shifting away from burning fossil fuels. (Presumably, humankind will have succeeded in switching to carbon-free energy sources during those 1000 years due to advances in technology—and because the world's supply of fossil fuels is finite.)

Making a Dent

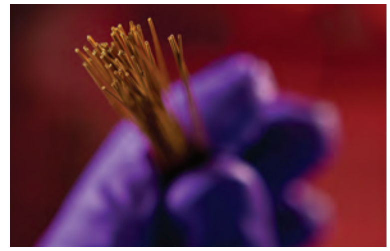
According to the Environmental Protection Agency, current annual CO_2 emissions in the United States are about six billion tonnes (metric tons: 1000 kg or 2205 lbs) out of about 30 billion tonnes worldwide. In order to contribute substantially to the solution, CCUS technology will eventually need to remove one billion tonnes of CO_2 per year worldwide. That would involve retrofitting existing power plants with carbon capture technology, building new plants with integrated capture technology, and constructing new pipelines to transport a volume of liquid CO_2 equal to about 35 percent of the world's oil production.

Still, with coal and other fossil fuel plants projected to continue to provide the majority of humanity's energy consumption for at least another 20 years, experts at Los Alamos and elsewhere are working to make CCUS as safe and economical as possible. A handful of existing CCUS pilot programs currently capture and store on the order of a million (not billion) tonnes of CO_2 per year, and a number of larger, industrial-scale CCUS projects are expected to be in operation in the United States and elsewhere by 2020. Then, in order to practically scale the collective tonnage up from millions to billions, three things will need to happen: larger geological repositories will need to be identified and tested, new pipelines and other infrastructure will need to be built, and the additional expense incurred due to CCUS activity per watt of energy produced will need to come way down. Finding suitable repositories may not be overly problematic, as deep saline aquifers are quite common and have an estimated worldwide capacity of ten *trillion* tonnes of CO_2. But reducing per-watt costs has proved significantly more challenging: the DOE target calls for 90 percent of all CO_2 generated by coal-based power production to be captured and stored at a maximum increase to the cost of electricity of 35 percent (for the least efficient existing power plants) and 10 percent (for newer, more efficient plants). Pilot programs don't even come close—not yet, anyway.

Creative Capture

Of all the CCUS activities—capture at the power plant, compression into fluid, transportation in pipelines, and underground injection and management—existing capture technologies account for upwards of 75 percent of the total expense. That capture expense is particularly large for our oldest, lowest-tech power plants, which require post-combustion carbon capture: the CO_2 must be separated and compressed from the plant's low-concentration, low-pressure exhaust gas—an energy intensive process. And the U.S. Energy Information Administration estimates that by 2030,

(Left) Kathryn Berchtold, team leader for Carbon Capture and Separations for Energy Applications at Los Alamos, and postdoctoral researcher Ganpat Dahe examine the hollow fiber membranes that she believes will ultimately be bundled into a commercially viable carbon capture module. (Below) Hollow fiber membranes for gas separation.



the current fleet of post-combustion power plants will still be responsible for 78 percent of the country's CO_2 emissions from electricity generation. Reducing capture costs at such plants constitutes the tremendous technological challenge facing Los Alamos's CaSEA team (carbon capture and separations for energy applications), led by Kathryn Berchtold.

Berchtold and her CaSEA colleague Rajinder Singh have been developing and experimenting with promising new membrane materials for inexpensively separating CO_2 from coal-derived gas streams produced during power generation processes. They aim to design, demonstrate, and ultimately commercialize a membrane-based separation process for both existing and next-generation power plants. That means identifying the best materials for the job and then maximizing throughput by laying those materials down in as thin a layer as possible without sacrificing structural integrity—hundreds of times thinner than a human hair. To that end, Berchtold and Singh have developed a novel ultrasonic atomization technology for depositing CO_2-selective layers onto a commercially viable, porous polymer film, which could then be rolled up for packaging and use. CaSEA scientists believe that the adaptability of this method will allow it to make that rare, but all-important, transition from the laboratory benchtop to real-world industrial use.

The CaSEA team is also pursuing separations technologies that meet the needs of more efficient, next-generation power plants. In these plants, a coal gasifier produces syngas: a mixture of hydrogen (H_2) and carbon monoxide (CO), plus other trace gases. The syngas is then reacted with steam, converting the CO to CO_2 while producing additional H_2. The H_2 is then separated from this mixed gas stream prior to its combustion. It burns cleanly and can be used as a transportation fuel or a source of electricity. All that remains is to compress the waste CO_2 and send it off to be injected deep underground.

One technology under development by the CaSEA team to separate H_2 from CO_2 comprises a special membrane material based on a commercially available chemical called polybenzimidazole (PBI) deposited on hollow-fiber support structures. These PBI-coated hollow fibers—roughly the diameter of a human hair—selectively allow the smaller H_2 molecules to pass into the hollow fibers while blocking the larger CO_2 molecules. Pressure and concentration gradients drive the separation.

"What's amazing about this PBI-based polymer is that it's stable at temperatures where most other polymers would degrade," Berchtold says. "This is a must for use at high gasification process temperatures. Matching the process and separation temperatures with a technology that's durable under those conditions is key to minimizing the cost of carbon capture." Indeed, the team's materials have proven extremely durable, outperforming all the other organic membranes identified for separating the syngas-derived mixture. Such membranes generally suffer from a trade-off: the better they are at distinguishing between the two gases, the lower their overall throughput. But the new PBI membrane shows a simultaneous improvement on both counts, and, as a consequence, Berchtold believes it finally puts the DOE's goal of capturing 90 percent of the CO_2 at only 10 percent increased cost of electricity within reach.

Heavy Metals in Concert

Back on the storage side, Los Alamos hydrogeologist Elizabeth Keating is asking a tough question: Could leakage of CO_2 from deep underground storage migrate upward, perhaps along undetected geologic faults or in leaking wells, and contaminate shallow-aquifer drinking water? Famous examples in France (where Perrier is bottled) show that carbonated water is not necessarily harmful. However, CO_2 may, in some circumstances, cause rocks in the aquifer to release toxic heavy metals into the drinking water. In addition, pressure in the storage reservoir may drive brine that contains heavy metals upward into the groundwater. These potentialities must be prevented, and that may not be easy.

Keating studies the CO_2-bearing groundwater at field sites she considers to be natural analogs to a leaking, large-scale carbon storage repository—sites where nature has provided migrating CO_2 within the geological strata through volcanic or other tectonic activity. (Sites of this sort would not be chosen for carbon storage operations.) One such site is just a 30-minute drive from Los Alamos, in Chimayó, New Mexico, where some locations have groundwater quality problems: the toxic elements arsenic and uranium are naturally present in the water. Keating samples groundwater and sediments over time for use in laboratory experiments, materials characterization, and computational modeling to determine how the natural CO_2 springs might contribute to the groundwater quality problems. She finds that brine accompanying the CO_2 as it rises from depth contains arsenic and uranium, while CO_2 reactions with aquifer rocks do not play an important role in releasing these elements.

"Because arsenic and uranium are strongly correlated with salinity at some of the wells," Keating says, "it's much more likely that brine from deep below, which is already rich in these metals, is coming up in those spots, too." If CO_2 storage operations cause a similar effect, it could become a deal-breaker for CCUS in general. Yet at other field sites, groundwater has proven to be well isolated from brine intrusion. Keating's research at a site in Springerville, Arizona, where CO_2 naturally enters the groundwater but metal-laden brine does not, may help identify why some locations are susceptible to brine entering shallow aquifers but not others.

Even without brine intrusion, what prevents CO_2 reactions with aquifer rocks from introducing toxic metals into the drinking water? Research at Chimayó by Keating and colleagues reveals an answer: minerals in the aquifer, such as iron-bearing clays, naturally draw the metals out of solution. This likely explains the absence of detectably elevated concentrations of arsenic or uranium in lower-salinity wells. It is not clear how quickly this process would remove toxic metals if a CO_2 storage reservoir were to leak, however, making further research essential.

To Seal the Deal

Of course, there is another concern, apart from groundwater contamination, associated with upward displacement from carbon storage sites. What if the CO_2 leaks back into the atmosphere? A large release could be life-threatening, displacing breathable oxygen from the air, but even a steady leak at nontoxic concentrations could undermine the purpose of the storage effort. Is there any way to verify that the captured gas won't just find its way out of the ground during its thousand years of intended containment?

Los Alamos scientists Dennis Newell and Bill Carey are trying to demonstrate just that. They argue that one of the most likely places to spout a significant leak is actually at the wellbores themselves. Whether designed for injection of CO_2, production of brine, or oil and gas operations, wellbores are plugged with cement across the deep caprock to isolate the CO_2 (or oil or gas) below from the groundwater above it and the surface. Even though many energy scientists expect that CO_2 injection will be a temporary measure—just until non-fossil-fuel energy sources can be widely deployed in 100 years, perhaps—the carbon must stay stored long after that, beneath a large number of sealed-off wellbores.

Newell and Carey recently performed a series of laboratory experiments designed to test wellbore seal integrity. They built a test seal between siltstone and cement to simulate a sealed wellbore but deliberately included a defect between the two layers. They then flooded it with a

(Left) The Arenal volcano in Costa Rica is an extreme example of a natural analog to a carbon storage site in which the CO_2 migrates upward to the surface. (Right) Los Alamos hydrogeologist Elizabeth Keating stands by a somewhat less dramatic natural analog, where underlying CO_2 ascends to the groundwater and the atmosphere at her field site in Chimayó, New Mexico.

CREDIT: (RIGHT) DANIEL LEVITT/LANL

high-temperature, high-pressure mixture of brine and supercritical CO_2 and measured the seal's permeability over time. Remarkably, that permeability decreased threefold over a period of days without any interference from the scientists.

"Based on our research, nature may be able to help with some of our problems," Newell says. "You've got a major leakage pathway in a mile-deep, manmade hole, and under some conditions, it actually heals itself. It is very important for us to identify the situations where self-healing can occur and those where it is unlikely." Detailed microscopic analysis revealed reactions of CO_2 with cement, showing where the brine-CO_2 fluid had migrated along the defect. Further evaluation of those penetration sites revealed that cement in the defect zone had been altered by the brine-CO_2 fluid and redeposited farther along in the defect, obstructing the leak.

For Carey, this is a gratifying result, because years of field-site leak testing have shown him that the cement interfaces are the most vulnerable parts of wellbore systems. If the self-healing behavior is found to be universal, or perhaps even inducible, he believes this will go a long way toward securing carbon storage reservoirs—an important step in making CCUS a reality.

Eyes and Ears on the Ground

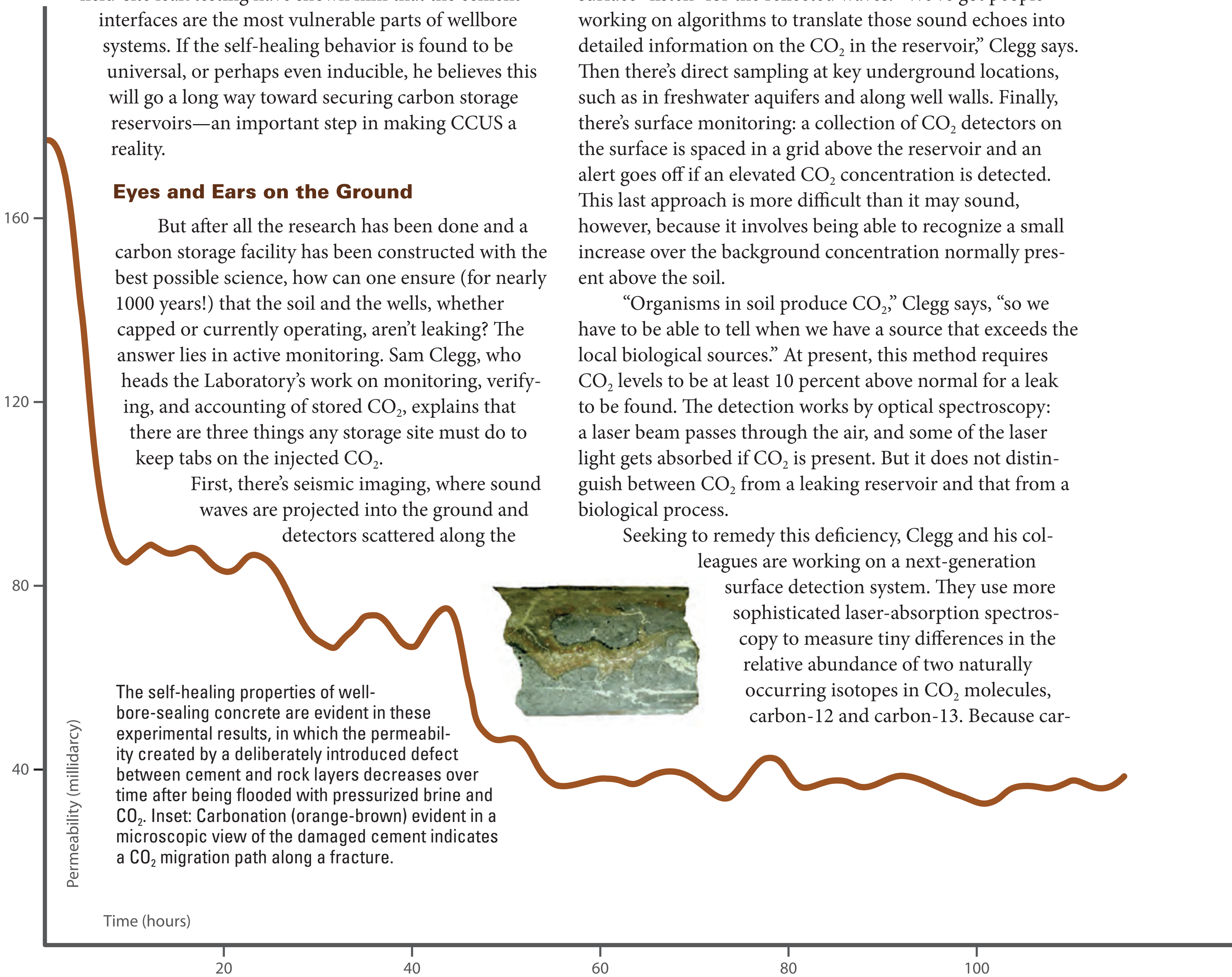
But after all the research has been done and a carbon storage facility has been constructed with the best possible science, how can one ensure (for nearly 1000 years!) that the soil and the wells, whether capped or currently operating, aren't leaking? The answer lies in active monitoring. Sam Clegg, who heads the Laboratory's work on monitoring, verifying, and accounting of stored CO_2, explains that there are three things any storage site must do to keep tabs on the injected CO_2.

First, there's seismic imaging, where sound waves are projected into the ground and detectors scattered along the surface "listen" for the reflected waves. "We've got people working on algorithms to translate those sound echoes into detailed information on the CO_2 in the reservoir," Clegg says. Then there's direct sampling at key underground locations, such as in freshwater aquifers and along well walls. Finally, there's surface monitoring: a collection of CO_2 detectors on the surface is spaced in a grid above the reservoir and an alert goes off if an elevated CO_2 concentration is detected. This last approach is more difficult than it may sound, however, because it involves being able to recognize a small increase over the background concentration normally present above the soil.

The 2010 Deepwater Horizon oil spill in the Gulf of Mexico is perhaps the best-known example of a wellbore failure—a phenomenon that Los Alamos scientists actively research in the context of keeping geologically stored CO_2 in the deep underground reservoirs where it was injected.

"Organisms in soil produce CO_2," Clegg says, "so we have to be able to tell when we have a source that exceeds the local biological sources." At present, this method requires CO_2 levels to be at least 10 percent above normal for a leak to be found. The detection works by optical spectroscopy: a laser beam passes through the air, and some of the laser light gets absorbed if CO_2 is present. But it does not distinguish between CO_2 from a leaking reservoir and that from a biological process.

Seeking to remedy this deficiency, Clegg and his colleagues are working on a next-generation surface detection system. They use more sophisticated laser-absorption spectroscopy to measure tiny differences in the relative abundance of two naturally occurring isotopes in CO_2 molecules, carbon-12 and carbon-13. Because car-



The self-healing properties of wellbore-sealing concrete are evident in these experimental results, in which the permeability created by a deliberately introduced defect between cement and rock layers decreases over time after being flooded with pressurized brine and CO_2. Inset: Carbonation (orange-brown) evident in a microscopic view of the damaged cement indicates a CO_2 migration path along a fracture.

bon-13 is heavier than carbon-12, it is used a little differently in chemical processes, manmade or otherwise. That difference is exaggerated in CO_2 produced by the burning of fossil fuels, producing a significant deficit in carbon-13 relative to that in CO_2 of biological origin. Together with seismic imaging and underground sampling, this surface detection system should eliminate the possibility of a leak going undetected.

Uplifting Prospects

Finding and exploring prospective storage sites is another research-intensive part of the CCUS initiative, and that's where Phil Stauffer, a Los Alamos hydrogeologist, comes in. Together with colleagues at the Laboratory and collaborators from the University of Wyoming, Stauffer has developed detailed computer simulations of a proposed CO_2 storage facility on the Rock Springs Uplift in southwestern Wyoming. The site has deep, porous limestone and sandstone layers amenable to carbon storage and is proximate to a coal-fired power plant that produces 18 million tonnes of CO_2 annually. The simulations show 50 years at 80 percent injection from the power plant (15 million tonnes per year) with minimal leakage into the caprock above and projected additional storage capacity for well over a century from all of the large CO_2-producing operations in southwestern Wyoming, amounting to about 30 million tonnes annually, roughly half of the state's total carbon emissions.

"We have new, high-resolution, 3-D seismic data that allows us to vastly improve our geologic models," Stauffer says. Together with a deep test well, a long core sample, and other sampling and analysis components, the new, data-rich simulation may allow the proposed facility to come to fruition. "We have transitioned from an idealistic, generalized assessment of the storage site to a realistic, low-risk assessment—one that finally justifies the investment to begin constructing a commercial storage operation."

Initially, the Rock Springs Uplift storage facility would span 100 square miles on the surface, requiring 26 injection wells and at least as many production wells, which make room for the injected supercritical fluid by drawing out the existing brine. These production wells are important because they reduce the pressure in the deep aquifer. This dramatically reduces the likelihood of excessive leaking, either upward or sideways beyond the footprint of the facility. It also significantly reduces the danger of triggering earthquakes due to overpressure, which could then lead to increased leakage. (Earthquakes have led to the cancellation of subsurface geothermal injection projects in Europe and the United States.)

A second benefit of extracting brine may come from the brine itself. During 50 simulated years of operation, approximately one cubic kilometer of simulated CO_2 was injected, resulting in about a cubic kilometer of simulated brine being produced. The large volume of very salty water, more than twice as salty as seawater, comes out of the ground at temperatures exceeding 100°C, making it a potentially useful source of geothermal energy. Additionally, the water could be desalinated for industrial or agricultural applications (if not for drinking), provided that the economic value of the produced freshwater justifies the expense of desalination. However, if desalination is not economically feasible, then proper disposal of the brine may prove difficult and expensive.

Stauffer's calculations make reasonable assumptions about well installation and operation costs. The proposed facility, he finds, would add only about one dollar to the cost of energy production per tonne of stored CO_2—a miniscule fraction of the cost of capturing the CO_2 from the power plant's exhaust to begin with.

Whether the Rock Springs Uplift plant goes forward or not, the DOE appears to be keeping up with its current timeline for developing and deploying CCUS technology. If surface and groundwater safety can be better assured and cost objectives met, then one or more full-scale demonstration facilities can begin on schedule in 2020. From there it will be a matter of improving the cost efficiency of capture technologies and scaling up overall deployment to the level where CCUS can make a serious dent in the emissions driving climate change.

With such a grand objective looming so near in the future, one might expect Rajesh Pawar and his colleagues around the country to feel a restless apprehension with every day that goes by. But in the wake of recent CCUS discoveries and achievements from Los Alamos, Pawar expresses optimism that the comprehensive effort to master this complex, new science can proceed as planned.

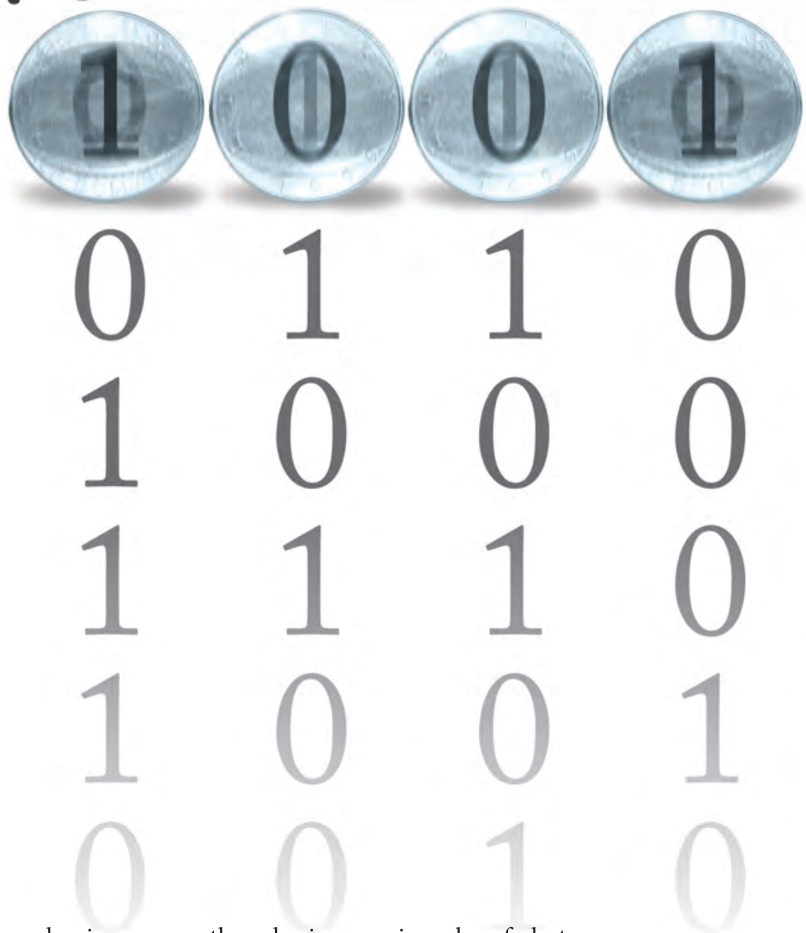
"Success in CCUS is all about removing the uncertainties," Pawar says, "and that's exactly what these projects are doing." ❖ LDRD

—Craig Tyler

The Jim Bridger coal-fired power plant lies on Southwestern Wyoming's Rock Springs Uplift, a promising site for a CO_2 storage operation.

Quantum DISCORD

A distinguishing trait of quantum correlations discovered at Los Alamos may be the key to a quantum leap in computing technology.



Quantum mechanics governs the submicroscopic realm of photons, electrons, and atoms. In principle, its equations are valid for an object of any size, but a large object (and large, in this context, could mean anything bigger than 10 or 20 atoms) cannot effectively be isolated from its environment because it undergoes incessant interactions with the matter and radiation surrounding it. A process called decoherence ensues: information describing the object's complex quantum state disperses into the environment, forcing the object into simpler states without the quantum features of its pre-decoherence state. Thus, even as the combined whole—object plus environment—adheres to the quantum rules of behavior, the object alone no longer exhibits any of the telltale signatures of quantumness and, in effect, "goes classical."

The border territory between quantum and classical is becoming increasingly important for applications, and Los Alamos National Laboratory Fellow Wojciech Zurek is making inroads into this regime. Zurek has dedicated much of his career to an elusive line of research into the foundations of quantum physics. How does the quantum behavior of the microscopic world give way to the classical behavior of the macroscopic world? Why do electrons behave differently than baseballs? Just where does that transition lie, and what rules emerge from it? What aspects of the world are irreducibly quantum?

Most of Zurek's work is foundational in nature, but just like the advent of quantum theory itself, which long preceded its many practical applications, his pure research now appears capable of sparking a revolution in technology. By characterizing the degree of quantumness inherent in a system of particles, he may have also provided a foundational element in the budding field of quantum computing, from which tremendous computational power can be unleashed if the quantum states of many particles can be mixed in such a way as to allow a large number of simultaneous calculations.

Such simultaneity has its roots in the fact that a quantum system can exist in a quantum combination of states known as a superposition. A simple example is the spin orientation of a single electron. As with any such "spin-½ system," an electron has two possible quantum states referred to as "up" and "down" with respect to any chosen axis. When the spin of an electron is measured, the result is always up or down and is never in between. But prior to that measurement, the electron can exist in a superposition of both states, and it is this superposition that gives rise to the possibility of quantum computation. The idea is to replace a classical bit of information, with a value of either 0 or 1, with a quantum bit, or qubit, in a superposition of both 0 and 1. Because each qubit simultaneously involves both 0 and 1, N qubits can simultaneously represent 2^N distinct possibilities. This quantum parallelism, if harnessed, could make certain types of computations much faster, accomplishing feats impossible for the fastest existing computers.

To appreciate the distinction between a quantum and classical computer, consider each performing a simulation of a quantum system consisting solely of spin-½ states. The powerful (but classical) Roadrunner supercomputer at Los Alamos has enough memory to store the state of a system containing at most 43 quantum spins, because 2^{43} (that's 8.8 trillion) complex numbers are needed to accomplish this. Simulating a complete quantum state of a system with one more spin—a collection of 44 electrons, say—would require doubling Roadrunner's size. Yet, in principle, a quantum computer consisting of just 44 qubits could do the same job.

The trick to practical quantum computation is to get many qubits to work together while being careful not to disturb them, because a disturbance would ruin their superposition the same way a spin measurement causes an electron spin to settle on a particular state—up or down and not both. But if avoiding a disturbance means perfectly isolating the qubits from the environment to prevent decoherence (decoherence which would, at best, turn the quantum computer into a poorly performing classical computer), then actually building a quantum computer would be nearly impossible.

The Entangled Web We Weave

Before the quantum computing community absorbed Zurek's foundational work, they assumed that getting qubits to work together to exploit quantum parallelism required "entangling" them. Entanglement occurs when two or more particles interact with one another and then remain correlated long after the interaction is over. For example, physicists can entangle two electrons so that they have opposite spins, while maintaining their superposition: once measured, one electron's spin will be up and the other will be down, but which one is which can only be settled by measuring one of them. Prior to that measurement, each electron has, in a sense, both spins. Thus, two entangled particles can share a correlated superposition of states. This is what quantum computers need: qubits to hold multiple values simultaneously (through superposition) and operate in coordination with other qubits (through entanglement).

Unfortunately, it has so far proven impractical to maintain entangled superpositions long enough to carry out any sizable quantum computation. Whenever any one qubit is disturbed (decohered by an air molecule, perhaps, or a stray photon of light), the entire entanglement collapses. And successful quantum computers capable of performing valuable tasks, such as detailed simulations for the development of advanced materials, would need to sustain thousands of entangled qubits such that none is disturbed.

The struggle to protect such a large-scale entanglement against an inescapable background of disturbances was

More than just answering a fundamental question— ***What makes a correlation quantum?****—quantum discord may provide the basis for significant technological progress.*

beginning to seem like a permanent deal-breaker until a proof-of-principle quantum computation was carried out using a less restrictive correlation among qubits than entanglement. That successful demonstration was based on Zurek's work.

When Mess is More

In 2000, Zurek proposed a new way to evaluate the quantumness of correlations between particles. He and Harold Ollivier, a graduate student who did part of his Ph.D. research with Zurek, used this new quantity to explore the effect of decoherence on quantum correlations. Zurek and Ollivier quantified the strength of the invisible quantum correlations by taking the quantum mutual information of a pair of qubits—a measure of how much the qubits "know" about each other—and subtracting from it the mutual information one would attribute to the pair if the correlation were classical. The result was dubbed discord. It quantifies the disagreement between the quantum and classical ways of calculating the same property.

Before discord, the sole criterion for the quantumness of correlation between particles was entanglement. All entangled states have discord. However, even when all entanglement has been eliminated by decoherence, Zurek and Ollivier showed, discord can still remain. Discord, then, measures how much of the correlation between particles is irreducibly quantum in nature. It is a more inclusive standard of correlation than entanglement, but because states that have substantial discord need not be entangled, it's also less sensitive to disturbances.

Zurek and Ollivier originally set out to explore the boundary between quantum and classical behavior using discord. The state of a pair of microscopic systems, such as entangled electrons with spins that are simultaneously up and down, is sharply changed by measurement and, therefore, the discord of an entangled electron pair is large. And a macroscopic object, such as a cup of coffee, is already decohered by the environment, so it doesn't observably change when something about it is measured; thus, its correlations with other objects have vanishing discord. But because the heart of a quantum computer lies in between these two extremes—it is "mesoscopic," perhaps, and very difficult to isolate from its environment to protect its entanglement—discord has helped restore the hope that such a computer can still be built.

Indeed, recent research has shown that quantum computing can be carried out without any entanglement, but in all such cases discord plays an important role. It is an open question whether quantum computing requires exactly the quantum correlation given by the formula for discord, but this question is now front and center, investigated in hundreds of scientific papers over the past few years. More than just answering a fundamental question—What makes a correlation quantum?—quantum discord may provide the basis for significant technological progress. A computer with qubits correlated by discord rather than entanglement requires less protection against external disturbances—and perhaps that difference will enable the first functioning prototype.

Now that discord has been shown to suffice for some types of quantum computation, researchers can focus on the question of why it suffices. Discord is a relatively new concept in quantum physics circles and has yet to be fully explored. Perhaps it will prove useful in many other contexts as well. Or maybe it's just a coincidence that it holds such practical value in this one. Regardless, Zurek hopes the recent focus on discord will lead to a deeper understanding of the quantum underpinnings of our world—and open the door to a quantum leap in technology. ❖ LDRD

—Craig Tyler

spotlights

Safer Nuclear Power

The worst nuclear accident in U.S. history took place in 1979 at the Three Mile Island (TMI) nuclear generating station in Pennsylvania. Radioactive gases were released, but the quantities were low enough that, evidently, no one was hurt. The more recent Fukushima disaster was similar to the TMI event, in that each was a loss-of-coolant accident (LOCA), which is essentially a plumbing problem: plant operators are unable to pump cool water through the reactor core, causing the core to get hotter and hotter. Even though any normal failure incident (faulty pump, earthquake, etc.) that could lead to a loss of coolant triggers a scram, in which control rods are inserted to halt the nuclear fission reactions, radioactive elements continue to generate heat inside the reactor as they decay.

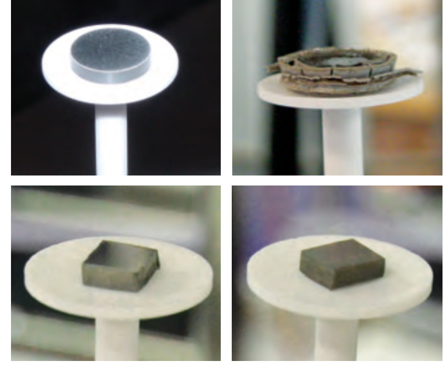
That by itself wouldn't be so bad—plant operators could just wait out the radioactive decay, after which the temperature would start to drop—if there weren't a second heat source inside the reactor. As the core temperature rises above a particular threshold, the thin tubes that encase each of the reactor's tens of thousands of fuel rods begin to oxidize, generating additional heat. Without cooling water, that additional heat continues to escalate temperatures, melting core components and eventually leading to containment failure and serious public health risk. Now, Los Alamos scientists, in collaboration with scientists from the Idaho and Oak Ridge national laboratories, are investigating a way to prevent that second heat source from kicking in.

The tube used to isolate the radioactive fuel from the water coolant, known as cladding, is usually made from a zirconium alloy chosen for its transparency to neutrons, because neutrons sustain the reactor's fission reactions under normal operating conditions. But when temperatures rise above 750°C under LOCA conditions, the zirconium undergoes a chemical reaction with the water (in the form of steam) that fills the reactor. The oxygen in the water reacts with zirconium metal to form zirconium oxide, which makes the cladding degrade and flake away. If this reaction continues, the highly radioactive fission products that were safely contained inside the cladding become free to mix with the water, greatly increasing the danger in the event of a loss of containment. Meanwhile, the hydrogen builds up pressure that could ultimately cause an explosion and breach of containment, as happened following the earthquake and tsunami at Fukushima. And because the reaction generates heat, once it begins, the reactor temperature will climb higher.

To prevent the reaction from starting in the first place, Los Alamos materials scientists Andrew Nelson and Stuart Maloy are using a novel experimentation platform to test zirconium and other cladding materials in the presence of steam at extremely high temperatures. Their experimental setup combines thermogravimetric analysis, which monitors the weight change as zirconium becomes zirconium oxide, with evolved gas analysis, which monitors the production of hydrogen.

They discovered, for example, that conventional stainless steel won't begin to oxidize until the temperature rises another 150° or so beyond the oxidation temperature for the zirconium alloy, up to 850–900°C. Therefore, if stainless steel were used to replace the zirconium alloy, it could buy plant operators more time to get cooling water into the reactor before it reaches the oxidation temperature. But without cooling water, the reactor will still reach that temperature following a typical LOCA.

"The explosion at Fukushima might have happened a few hours later with conventional stainless steel cladding," Nelson says, "but it still would have happened."



(Upper row) Zirconium alloy test sample before (left) and after (right) being damaged by temperature and steam conditions typical of a loss-of-coolant accident in a nuclear reactor. (Lower row) PM2000 metal before (left) and after (right) being subjected to the same conditions.

CREDIT: ANDREW NELSON/LANL

However, when Nelson and Maloy tested a commercial variety of stainless steel enriched with aluminum, known as PM2000, they found that the oxidation reaction didn't generate significant heat up to 1200°C—at least 200° hotter than a reactor undergoing a TMI- or Fukushima-type LOCA should get from radioactive decay heat alone. Furthermore, the oxide formed by the reaction was protective; it did not flake off. This could be game-changing: if PM2000 cladding is used, LOCAs like these should no longer lead to explosion or meltdown, and radioactive material will not get out. More research is needed, however, to test the corrosion and radiation resistance of PM2000 under long-term reactor use. And procedures need to be developed for producing thin tubes and making sound welds from the alloy.

Will this discovery improve nuclear power safety under accident conditions? "It will certainly be much safer," answers Nelson, who argues that nothing can make it 100 percent safe. "PM2000 cladding won't save you if the reactor is hit by a meteor." Yet, cosmic collisions aside, commercial adoption of cladding made from PM2000 or a similar alloy may depend upon an economic question: will nuclear fuel vendors be able to recover the R&D costs of developing these new fuel rods? Nelson, who collaborates on this issue with the two largest U.S. vendors, General Electric and Westinghouse, is hopeful that the answer is yes and that safer nuclear power—using existing power plants—really is on its way. Because PM2000 is also likely to withstand normal operating conditions better than zirconium alloy, power plants may be able to operate their reactors for longer periods of time between refueling and maintenance shutdowns. And more time online is more time earning revenue.

—Craig Tyler

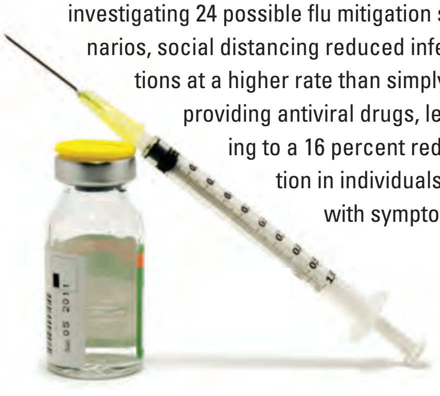
Preventing a Pandemic

The H1N1 influenza outbreak during 2009 was the first new flu strain with global reach in 40 years, and its initial virulence alarmed public health officials. As the pathogen spread from Mexico to the U.S. in early spring, the Department of Homeland Security hired a team from Los Alamos, Argonne, and Sandia national laboratories to simulate the pandemic in the United States.

Influenza outbreaks are a combination of unpredictable human and virus behavior, so they are fraught with uncertainty. The outcome of H1N1 was less severe than past flu pandemics, but Los Alamos-led research now explains how much worse it could have been. Understanding how scenarios based on the potential range of uncertainties could unfold will help federal and local agencies stockpile vaccines and antiviral drugs to plan for future worst-case events.

The Critical Infrastructure Protection and Decision Support Systems (CIPDSS) research team used infrastructure models combined with a general infectious disease model to study an additional element of the pandemic—how absence from work during an outbreak affects the economy. Specifically, the team's simulation involved a public health strategy called "social distancing," in which people who feel well avoid work and school.

In a recent publication of the 2009 study investigating 24 possible flu mitigation scenarios, social distancing reduced infections at a higher rate than simply providing antiviral drugs, leading to a 16 percent reduction in individuals with symptoms.



However, that mitigation strategy was costly. There was a 50 percent decrease in gross domestic product over the course of the epidemic due to worker absences.

The CIPDSS team, including Rene LeClaire, Dennis Powell, Leslie Moore, Lori Dauelsberg, and others, also found that keeping kids from school during the modeled pandemic didn't entirely squelch the disease but did delay it. That technique could give researchers several months to develop or accumulate vaccines and antiviral drugs. "We're just trying to buy time through hand washing and social distancing while we're making the vaccine," said Jeanne Fair, infectious disease expert at Los Alamos and lead analyst for the project.

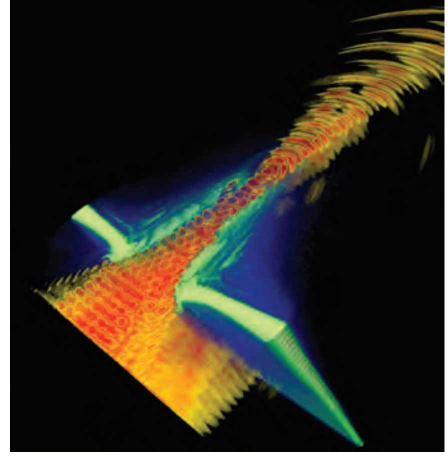
While H1N1 wasn't as devastating as public health officials feared, Fair says the analysis demonstrates the need to remain vigilant against future contagions. The worst-case scenario in the study could have four times more flu-caused fatalities in the United States than the estimated 675,000 (and perhaps 50 million worldwide) from the 1918 outbreak, which is the most severe flu pandemic on record.

—Sarah Keller

Laser Clarity

More than 50 years ago, scientists predicted that a laser could generate ions by driving the electrons in plasma to near the speed of light. Plasma typically reflects laser light, but when a strong laser accelerates electrons in the charged gas, plasma can become transparent. During this phenomenon called relativistic transparency, the laser's energy is transferred to electrons in the plasma, which in turn energizes ions. Until recently, researchers could only test the fundamental physics of relativistic transparency in computer simulations.

In research published last summer, plasma physicists at Los Alamos, along with collaborators in Germany and the United Kingdom, observed the dynamics of relativistic transparency for the first time. To do so,



In this research simulation of relativistic transparency, Los Alamos's Trident laser (orange) penetrates a 100-nanometer-thick carbon nanofoil (green). This generates a plasma, which typically reflects laser light like a mirror. Shown here, however, the strong laser drives the plasma electrons to near the speed of light, making the plasma transparent to the laser. Los Alamos plasma physicists have observed the dynamics of this for the first time.

CREDIT: DANIEL JUNG AND HUI-CHUN WU/LANL

they directed the Laboratory's 200 trillion-watt peak power short-pulse TRIDENT laser at 10- to 100-nanometer thick carbon foils to generate an electron-rich, transparent plasma. The team's new understanding of the relativistic transparency can be applied to developing laser-driven particles accelerators, x-ray sources, and ions for cancer treatment.

Relativistic transparency happens in a tenth of a picosecond, about the time it takes light to travel 1/30th of a millimeter. Previous studies had much lower time resolution, which limited how well researchers could understand the process. The new results will help advance work to precisely control the shape and timing of laser pulses, which is necessary for developing laser-driven particle accelerators that are smaller and less expensive than conventional accelerators.

The team found close agreement between current laser-plasma interaction models and their experiments, which confirms what Los Alamos scientists have long suspected—that directing a short-pulse laser at a very thin carbon foil target will make the foil transparent to the laser. "It validates the simulation code that researchers have been using for some time," said Sasi Palaniyappan of the Los Alamos plasma physics group. "At the same time it also tells us that we're doing an experiment that's as close as possible to simulation."

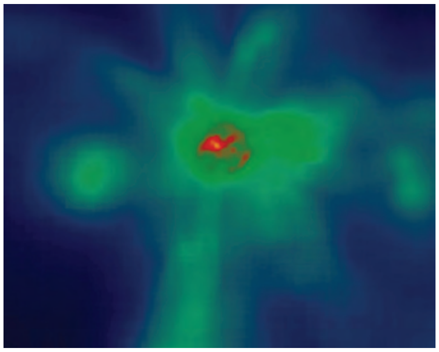
Researchers are investigating energetic ions, like those created during relativistic transparency by compact, high-powered lasers, as alternatives to traditional radiation therapy for cancer. The plasma physics team at Los Alamos is currently using TRIDENT for basic physics research to explore how to achieve the ion properties required for cancer treatment using laser-based ion acceleration. ❖ LDRD

—Sarah Keller

Great Balls of Fire

The largest black holes in the universe, known as supermassive black holes (SMBHs), are found at the centers of galaxies and can have billions of times the mass of the Sun (billions of solar masses). But black holes are created by the deaths of massive stars, and the largest known black hole birth weight is only a little over 20 solar masses. Astronomers presumed that although black holes were born small, they grew more massive over time by pulling in nearby gas. As the reasoning went, in a universe 14 billion years old, supermassive holes had lots of time to become supermassive.

However, telescopic observations, particularly in the last decade, have cast doubt on that reasoning. Quasars, distant light sources produced by hot gas flowing onto SMBHs, have now been detected at such great distances that their observed light began its journey to Earth when the universe was less than a billion years old. And the SMBHs at the heart of these quasars were already billions (10^9) of solar masses at that time. The most distant known quasar is powered by a two-billion solar mass SMBH seen when the universe was only six percent of its present age. How could stellar-mass black holes have grown to become supermassive in so little time? Black hole growth rates are limited because when they grow too quickly, the gas near the hole becomes so bright that it pushes the surrounding gas away, reducing the hungry hole's food supply.



In this simulation, a black hole that was just formed by the collapse of a supermassive star is surrounded by a distribution of gas (color indicates density). Because the black hole (located at the center but too small to see) grows by consuming the available gas, simulations like this one help determine how quickly the black hole can grow. The progenitor of this black hole, which contained up to a hundred thousand suns' worth of mass in a single star, could only have formed in the very early universe.

CREDIT: JARRETT JOHNSON/LANL

Los Alamos astrophysicist Jarrett Johnson thinks the first SMBHs in the universe had a head start. Supermassive holes, he claims, begin with supermassive stars (SMSs)—hypothetical objects containing up to about a million (10^6) solar masses in a single star. Normally, stars can't become supermassive because the gas clouds from which they form become clumpy as they collapse, fragmenting the cloud into many smaller stars. The gravitational collapse of a large gas cloud, therefore, results in a cluster of stars, typically less than one solar mass, with perhaps a few exceeding 100 solar masses—well short of the supermassive.

But things were different in the universe's first billion years, Johnson says. "In order for gas clouds to fragment into many stars, you need atoms and molecules to radiate away the heat from the collapse, forming cooler pockets. But sometimes these atoms and molecules just weren't there." Indeed, without sufficient cooling, higher temperatures meant higher pressures, inhibiting the collapse of gas into stars. And elements heavier than helium—those capable of providing cooling—were rare back then because they are only synthesized inside stars, and few stars yet existed. Thus with only two elements available, hydrogen and helium, there weren't many ways to radiate heat away from a gas cloud. And although molecules, including H_2, can cool regions within a larger cloud, such molecules could be dissociated into separate atoms in the presence of sufficient radiation. Without any way to cool distinct regions within the cloud, the whole thing could collapse under gravity's relentless force into a single, supermassive star. And when an SMS dies, less than a million years after its birth, its core forms a black hole that consumes most of the star, resulting in an instant 10^5 or 10^6 solar mass black hole.

Most astronomers have found this scenario unlikely, doubting that large regions could be flooded with enough molecule-dissociating radiation, sustained long enough to grow SMSs. But Johnson's research says otherwise. Together with collaborators from the Max Planck Institute in Germany, he performed large-scale cosmological simulations to search for the emergence of star-forming gas clouds embedded in a bath of molecule-dissociating radiation. Such conditions, he discovered, occur much more often than previously expected. In addition, he and Los Alamos colleagues Dan Whalen, Chris Fryer, and Hui Li modeled the conditions under which an SMS would form and found growth rates that similarly exceeded expectations: Once the collapse progresses to the point where the star "turns on," it continues to grow from rapidly infalling gas. The rate of infall is limited by the bright starlight that tends to push the gas away, but nonetheless, he found that accumulations up to about 10^6 solar masses are possible by the time the star dies and becomes a black hole.

Johnson is gratified with his results. "The emergence of billion-solar-mass black holes in the first billion years has been a major mystery in astrophysics," he says. "I think we finally have a plausible explanation." Johnson's work shows the validity of SMS formation—perhaps even widespread SMS formation—in the early universe, providing a much-needed way to kick-start the growth of SMBHs. Better still, if he's right, then ancient SMSs should be observable for the first time with the James Webb Space Telescope, Hubble's successor, which is planned for launch in 2018. ❖ LDRD

—Craig Tyler

ISSN: 1942-6631

Address mail to:
1663
Mail Stop M711
Los Alamos National Laboratory
P.O. Box 1663
Los Alamos, NM 87545
Email: 1663magazine@lanl.gov
Fax: 505-665-4408
www.lanl.gov/science/1663/

Presorted Standard
U.S. Postage Paid
Albuquerque, NM
Permit No. 532

Winter in the mountains of Northern New Mexico

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by Los Alamos National Security, LLC, for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396.
A U.S. Department of Energy Laboratory LALP-13-003